(4)

CHEMICAL RESEARCH, DEVELOPMENT & ENGINEERING CENTER

CRDEC-TR-168

COMPUTER-ASSISTED DETERMINATION OF MINIMUM ENERGY CONFORMATIONS IV. ALPHA1 AND ALPHA2 ADRENERGIC COMPOUNDS

William P. Ashman
Alexandar P. Mickiewicz

RESEARCH DIRECTORATE

June 1990

U.S. ARMY
ARMAMENT
MUNITIONS
CHEMICAL COMMAND

Aberdeen Proving Ground, Maryland 21010-5423

Disclaimer

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorizing documents.

Distribution Statement

Approved for public release; distribution is unlimited.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	1990 June	Final, 88 Jan - 89 Feb

4. TITLE AND SUBTITLE
Computer-Assisted Determination of Minimum Energy Conformations IV. Alpha1 and Alpha2 Adrenergic Compounds

5. FUNDING NUMBERS
PR-1C162622A554

6. AUTHOR(S)
Ashman, William P., and Mickiewicz, Alexander P.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
CDR, CRDEC, ATTN: SMCCR-RSP-C, APG, MD 21010-5423

8. PERFORMING ORGANIZATION REPORT NUMBER
CRDEC-TR-168

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

Conformational minimum energy calculations were performed on three-dimensional representations of 56 selected adrenergic compounds to achieve molecular-mechanics structure optimization (optimized geometries) using the empirical Molecular Mechanics II (MM2) computer program developed by Allinger and Yuh. Three-dimensional Cartesian atom coordinates for the minimum energy conformation of the 56 adrenergic compounds are reported. The calculated optimized geometries results can be used as initial structural configurations in future structure-activity relationships and molecular-modeling studies of adrenergic compounds.

14. SUBJECT TERMS			15. NUMBER OF PAGES
Minimum energy conformation,	Chemical compounds,	MM2	76
3-Dimensional coordinates,	Alpha1 adrenergic		16. PRICE CODE
Structure-activity relationship,	Alpha2 adrenergic		
	Molecular modeling		

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

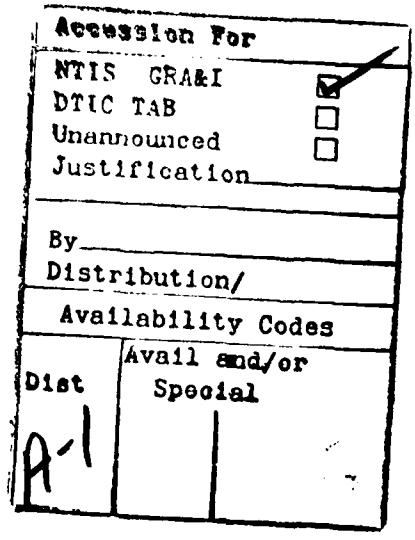
Blank

PREFACE

The work described in this report was authorized under Project No. 1C162622A554, Chemical Munitions. This work was started in January 1988 and completed in February 1989.

The use of trade names or manufacturers' names in this report does not constitute an official endorsement of any commercial products. This report may not be cited for purposes of advertisement.

This report has been approved for release to the public.



Blank

CONTENTS

Blank

COMPUTER-ASSISTED DETERMINATION OF MINIMUM ENERGY CONFORMATIONS
IV. ALPHA1 AND ALPHA2 ADRENERGIC COMPOUNDS

1. INTRODUCTION

Adrenergic compounds[1-10*] are classified by their interaction with specific adrenoreceptor types. Timmermans review[2] discusses the various adrenoreceptors and the activity that results when a compound interacts with a specific class. Adrenoreceptors are located in various locations within the body (i.e., central nervous system, fat cells, smooth muscle tissue, and platelets);[2] and the physiological activity of adrenoreceptors includes control of vasoconstriction, control of neurotransmitters (norepinephrine), and inhibition of sympathetic tone. The above activities can result in hypotension, sedation, and bradycardia.

Compounds that interact with adrenoreceptors display agonist or antagonistic action with the specific adrenoreceptor due to the physiochemical, geometric, and electronic characteristics of their molecular structure. This report discusses adrenergic compounds that act on alphal and alpha2 type adrenoreceptors. Specifically, the three-dimensional geometric coordinates are defined.

Research is ongoing to design and test adrenergic compounds for therapeutic use.[1-10*] New adrenergic compounds are designed using computer-assisted technology to direct the synthesis of compounds and to determine what physiochemical, geometrical, and electronic parameters relate to the resultant activity of the compound. The analysis of these parameters result in structure-activity relationship (SAR) models that lead to new compounds with the desired physiological response.

An important parameter in the development of SAR models that correlate compound-receptor interaction is the 'shape' of the molecule.[11] Previous reports[12-14] in this series discussed the theoretical perspectives and general methodology used to optimize chemical structures and define their minimum energy conformation or 'shape.' This same methodology was used in the analysis of the 56 adrenergic compounds studied in this report. The Molecular Modeling, Analysis and Display System (MMADS)[15] was used to construct the compounds, modify the conformations, and calculate the three-dimensional minimum energy coordinates. X-ray crystal atomic coordinates were used as starting conformations for noradrenaline[16] and clonidine.[17]

This report gives the compounds' three-dimensional Cartesian atom coordinates that can be used as initial structural configurations for use in future structure-activity relationship and molecular-modeling studies.

---

*Ashman, W.P., and Mickiewicz, A.P., "Structural Conformation Designed for use in Structure Activity Analysis," U.S. Army Chemical Research, Development and Engineering Center, June 1990, unpublished data.

2. ADRENERGIC COMPOUND STRUCTURES

Two-dimensional structural drawings of 56 adrenergic compounds (see Table 1) were obtained from various sources.[1-10]* These two-dimensional representations defined the initial structures that were incorporated into MMADS for threedimensional conformation analysis.

3. THREE-DIMENSIONAL MINIMUM ENERGY CONFORMATION OPTIMIZATION

Conformational minimum energy calculations were performed to achieve molecular mechanics structure optimization[18] (optimized geometries) using the empirical Molecular Mechnics (MM2) (QCPE Version dated 1980) computer program developed by Allinger and Yuh.[19] The Chemometric/Biometric Modeling Branch, Research Directorate, U.S. Army Chemical Research, Development and Engineering Center, MMADS (Version 3.1) was used to incorporate the adrenergic structures and perform the minimum energy calculations.

Initial conformations were constructed by orienting atom chains and atom rings in various combinations of otrans, cis, and gauche conformations. Dihedral angles for atom rings and substituent atom chains were rotated every 30°. For each 30° increment, energy minimizations were performed to differentiate between local minima. After finding the smallest local minima, the substituent groups and rings were then rotated at smaller degree increments until the optimum minimum energy conformation was obtained.

Every effort was made to locate the minimum energy conformation for the adrenergic compounds studied. However, the possibility exists that a lower minimum, than the final one reported, can be found in the conformational space investigated. The lowest local minimum calculated was reported as the resultant MM2 value for the optimized geometry for the three-dimensional coordinates calculated. This geometric conformation is recommended for use as the initial configuration for analysis.

The parameter set supplied with the MM2 program was used when required for structure-geometry optimization. If required, special parameters for atom bond lengths and angles and torsional angles were not available within the MM2 program, parameters for atom -atom interactions were calculated using the ab initio GAUSSIAN82[20] program and/or parameters were theoretically estimated.** Appendix A contains a set of parameters that when added to previously published parameters[13] can be used to calculate the MM2 minimum energy conformations of the adrenergic compounds of this report.

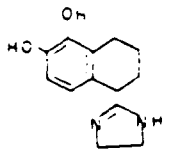
Computer-assisted determination of minimum energy conformations was executed on a Digital Equipment Corporation (DEC) (Maynard, MA) MicroVax II within a MicroVMS operating system environment. Tektronix 4105 series color

---

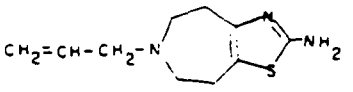
*Ashman, W.P., and Mickiewicz, A.P., "Structural Conformation Designed for use in Structure Activity Analysis," U.S. Army Chemical Research, Development and Engineering Center, June 1990, unpublished data.

**Ashman, W.P., U.S. Army Chemical Research, Development and Engineering Center, June 1990, unpublished data.

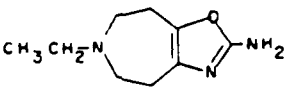
Table 1. Two-Dimensional Structure Representation of Adrenergic Compounds



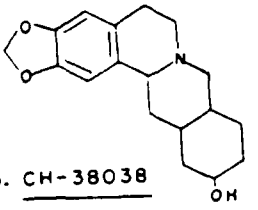
1. A2AGON



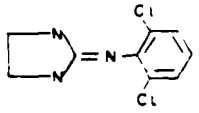
2. BHT920 & 3. BHT9201N



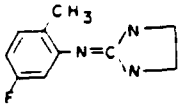
4. BHT9331N



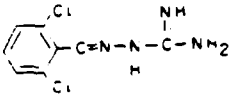
5. CH-38038



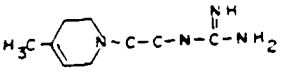
6. CLONIDINE



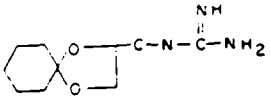
7. FLUTONIDINE



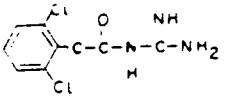
8. GUANABENZ



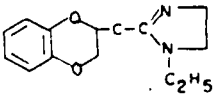
9. GUANACLINE



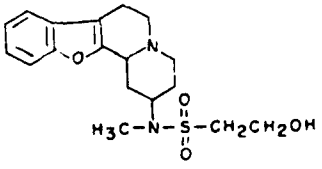
10. GUANADREL



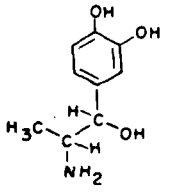
11. GUANFACINE



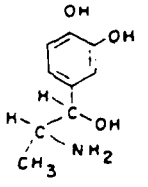
12. IMILOXAN (RS 21361)



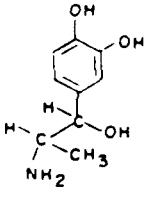
13. L654284



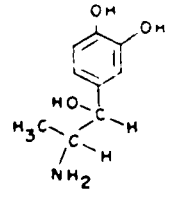
14. METHNOR1R2R



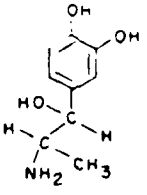
15. AMETHNOR1R2S



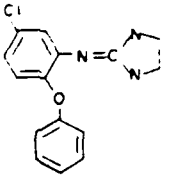
16. AMETHNOR1R2SNH2



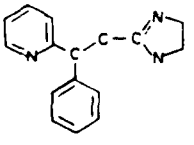
17. AMETHNOR1S2R



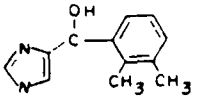
18. AMETHNOR1S2S



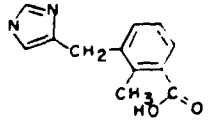
19. MIDAGAA



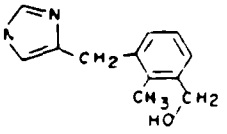
20. MIDAGLIZOLE



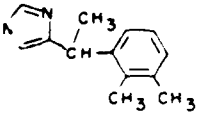
21. MPV1



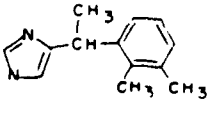
22. MPV1180



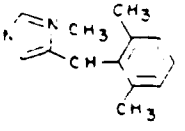
23. MPV1181



24. MPV1440

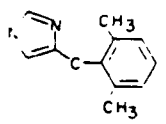


25. MPV785

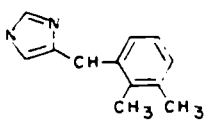


26. MPV2

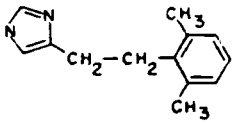
Table 1. Two-Dimensional Structure Representation of Adrenergic Compounds (Continued)



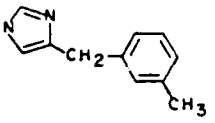
27. MPV 207



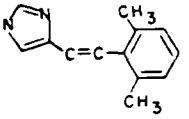
28. MPV 253



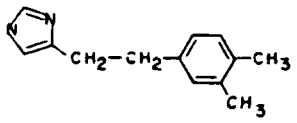
29. MPV 295 B
30. MPV 295A



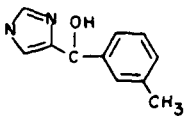
31. MPV 3



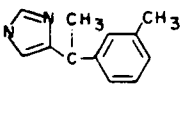
32. MPV 305T



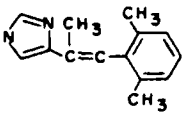
33. MPV 327 B
34. MPV 327A



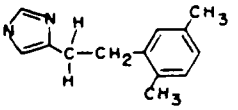
35. MPV 4



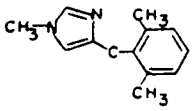
36. MPV5 B
37. MPV5A



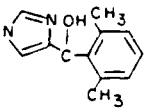
38. MPV 7



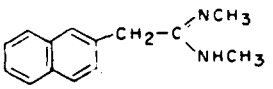
39. MPV 743



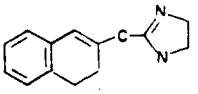
40. MPV 750



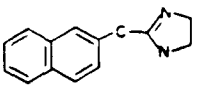
41. MPV 830



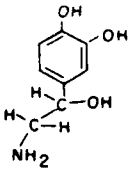
42. NAPACTADINE



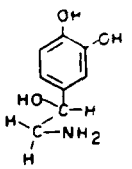
43. NAPAMEZOLE



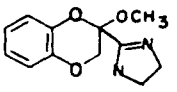
44. NAPAPHEN



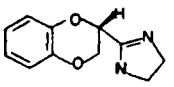
45. NORADIR



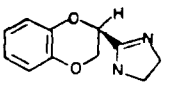
46. NORADIS



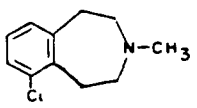
47. RX821002S



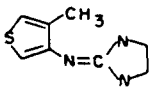
48. RX781094S



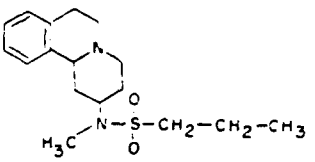
49. RX781094R



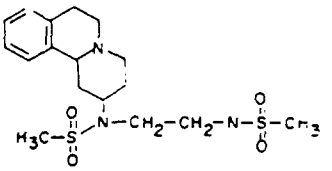
50. SKF86466



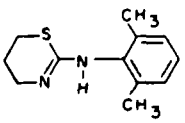
51. TIAMENIDINE



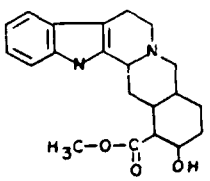
52. WY 26392



53. WY 27127



54. XYLAZINE B
55. XYLAZINE A



56. YOHIMBINE

graphics computer terminals were used, and an Adage 3000 raster display system provided high resolution graphics capability.

4. RESULTS

The MM2 calculated minimum energy corresponding to the optimized structure geometry and the adrenergic activity (if available) for the 56 adrenergic compounds are contained in Table 2. The adrenergic activity refers to the interaction of the compound with alphal and/or alpha2 adrenergic receptors and whether the compound is agonistic or antagonistic.

The individual compound structure files that list the MM2 program-calculated three-dimensional Cartesian atom coordinates cooresponding to the minimum energy optimized geometry are reported in Appendix B.

The resultant optimized geometries can be used as initial structural configurations for use in future structure-activity relationship and molecular modeling studies.

It should be noted that the MM2 minimized structures of clonidine and noradrenaline differed from the x-ray crystal conformations. An analysis of the noradrenaline structures (Norad1R and Norad1S) having the NH2 group of noradrenaline in a trans extended conformation (x-ray - Norad1R) versus the NH2 group rotated 120° (Norad1S), indicates that the MM2 minimum energy of the trans extended conformation is higher than the rotated MM2 conformation. This NH2 rotation may play an influence on the interaction of the compound with the adrenergic receptor, and erroneous conclusions may be made if one does not consider this conformation difference in structure-activity analyses. The MM2 energy difference is only 0.25 kcal, which is a very small difference, and the possibility of rotation from the trans extended form is reasonable. Therefore, in performing pharmacophore structure-activity studies, the researcher should use the conformations reported as initial structures and also rotate groups within molecules to potential overlapping positions with other molecules being studied.

Table 2. MM2 Molecular Mechanics Energy and Alphal and Alpha2 Adrenergic Receptor Activity

NO.	STRUCTURE NAME	ADRENERGIC ACTIVITY			MOLECULAR MECHANICS
		ALPHA1	ALPHA2	BOTH	ENERGY (kcal)
1.	A2AGON (1)		a	a	15.30
2.	BHT920 (2)		a		23.67
3.	BHT9201N (2)		a		23.61
4.	BHT9331N (3)		a		23.69
5.	CH-38038 (4)		b		36.18
6.	CLONIDINE (2)	a	a	a	27.18
7.	FLUTONIDINE (3)				12.65
8.	GUANABENZ (2)		a		23.00
9.	GUANACLINE (5)				9.33

Table 2. MM2 Molecular Mechanics Energy and Alpha1 and Alpha2 Adrenergic Receptor Activity (continued)

NO.	STRUCTURE NAME	ADRENERGIC ACTIVITY ALPHA1	ALPHA2	BOTH	MOLECULAR MECHANICS ENERGY (kcal)
10.	GUANADREL (5)				17.83
11.	GUANFACINE (2)	a	a	a	18.27
12.	IMILOXAN (4)		b		19.52
13.	L654284 (6)		b		29.59
14.	METHNOR1R2R (7)				3.23
15.	AMETHNOR1R2S (7)		a	a	3.09
16.	AMETHNOR1R2SNH2 (7)		a	a	3.88
17.	AMETHNOR1S2R (7)		a	a	3.69
18.	AMETHNOR1S2S (7)				3.05
19.	MIDAGAA (4)	b			13.11
20.	MIDAGLIZOLE (4)		b		24.97
21.	MPV1 (8)	a	a	a	16.10
22.	MPV1180 (9)				16.52
23.	MPV1181 (9)				17.07
24.	MPV1440 (8)		a		20.39
25.	MPV785 (8)				19.61
26.	MPV2 (*)				21.59
27.	MPV207 (8)				16.62
28.	MPV253 (9)				17.08
29.	MPV295 (8)				16.77
30.	MPV295A (8)				16.74
31.	MPV3 (*)				14.84
32.	MPV305T (8)				25.72
33.	MPV327 (9)				15.01
34.	MPV327A (9)				14.99
35.	MPV4 (*)				13.58
36.	MPV5 (*)				16.82
37.	MPV5A (*)				16.89
38.	MPV7 (*)				40.88
39.	MPV743 (9)				15.08
40.	MPV750 (9)				17.95
41.	MPV830 (8)				16.31
42.	NAPACTADINE (4)		b		0.07
43.	NAPAMEZOLE (4)		b		13.34
44.	NAPAPHEN (*)				5.84
45.	NORAD1R (7)	a		a	2.36
46.	NORAD1S (7)			a	2.11
47.	RX821002S (4)		b		21.72
48.	RX781094S (2)		b		19.79
49.	RX781094R (2)		b		15.52
50.	SKF86466 (10)		b		16.86

*Ashman, W.P., and Mickiewicz, A.P., "Structural Conformation Designed for use in Structure Activity Analysis," U.S. Army Chemical Research, Development and Engineering Center, June 1990, unpublished data.

Table 2. MM2 Molecular Mechanics Energy and Alpha1 and Alpha2 Adrenergic Receptor Activity (continued)

NO.	STRUCTURE NAME	ADRENERGIC ACTIVITY			MOLECULAR MECHANICS
		ALPHA1	ALPHA2	BOTH	ENERGY (kcal)
51.	TIAMENIDINE (3)				17.16
52.	WY26392 (4)		b		28.44
53.	WY27127 (4)		b		32.13
54.	XYLAZINE (2)	a	a	a	3.05
55.	XYLAZINEA (2)	a	a	a	2.94
56.	YOHIMBINE (2)		b		41.69

a = agonist
b = antagonist

Blank

LITERATURE CITED

1. DeBarnardis, J.F., Kerkman, D.J., Arendsen, D.L., Buckner, S.A., Kyncl, J.J., and Hancock, A.A., "Conformationally Defined Adrenergic Agents. 5. Resolution, Absolute Configuration, and Pharmacological Characterization of the Enantiomers of 2-(5,6-Dihydroxy-1,2,3,4-tetrahydro-1-napthyl)imidazoline: A Potent Agonist at alpha-Adrenoreceptor," Journal of Medicinal Chemistry Vol. 30, pp 1011-1017 (1987).

2. Timmermans, P., and van Zwie, P.A., "alpha2-Adrenoreceptors: Classification, Localization, Mechanisms, and Targets for Drugs," Journal of Medicinal Chemistry Vol. 25 (12), pp 1389-1401 (1982).

3. Kobinger, W., "Drugs as Tools in Research on Adrenoreceptors," Archives of Pharmacology Vol. 332, pp 113-123 (1986).

4. Luttinger, D.L., and Hlasta, D.J., "Antidepressent Agents," Annual Reports in Medicinal Chemistry Vol. 22, p 27 (1987).

5. Merck Index, 10th ed., Merck & Co., Rahway, NJ, 1983.

6. Pettibone, D.J., Clineschmidt, B.V., Lotti, V.J., Baldwin, J.J., Huff, J.R., Randall, W.C., Vacca, J., and Young, S.D., "Pharmacological Profile of a New Potent and Specific Alpha2 Adrenoreceptor Antagonist, L-657,753," Naunyn-Schmiedeberg's Archives of Pharmacology Vol. 336, pp 169-175 (1987).

7. Ruffolo, R.J., "Stereochemical Requirements for Activation and Blockade of Alpha1- and Alpha2- Adrenoreceptors," Trends In Pharmaceutical Science, pp 160-164.

8. Savola, J., "alpha-Adrenoreceptor Activity of Arylalkylimidazoles Is Improved by Alpha-methylation and Impaired by alpha-Hydroxylaion," Archives of Pharmacology Vol. 334, pp 423-429 (1986).

9. Vakkuri, O., Salonen, J.S., Leppaluoto, J., Antitila, M., Darjalainen, A., and Jarvensivu, P., "Radioimmunoassay of Detomidine, A New Benzylimidazole Drug With Analgesic Sedation Properties," Life Sciences Vol. 40, pp 1357-1364 (1987).

10. Sugrue, M.F., and Smith, R.L., "Chapter 9. Antiglaucoma Agents," Annual Reports in Medical Chemistry Vol. 20, p 85 (1985).

11. Hopfinger, A.J., "A QSAR Investigation of Dihydrofolate Reductase Inhibition by Baker Triazines Based Upon Molecular Shape Analysis," Journal of the American Chemical Society Vol. 102, pp 7196-7206 (1980).

12. Davis, E.G., Ashman, W.P., Mickiewicz, A.P., Lewis, J.H., and Thompson, J.H., Computer-Assisted Determination of Minimum Energy Conformations, I. Investigation of Selected 3-Azabicyclo[3.3.1]nonane Compounds, CRDEC-TR-88123, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, July 1988, UNCLASSIFIED Report.

13. Davis, E.G., Ashman, W.P., and Mickiewicz, A.P., Computer-Assisted Determination of Minimum Energy Conformations, II. Investigation of Selected Azabicyclononane and Azabicyclooctane Compounds, CRDEC-TR-88169, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, January 1989, UNCLASSIFIED Report.

14. Ashman, W.P., Mickiewicz, A.P., and Davis, E.G., Computer-Assisted Determination of Minimum Energy Conformations, III. Investigation of Selected G-Type Organophosphorous Compounds, CRDEC-TR-88170, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, January 1989, UNCLASSIFIED Report.

15. Leonard, J.M., A User's Guide to the Molecular Modeling, Analysis, and Display System (MMADS), CRDEC-TR-86039, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, May 1986, UNCLASSIFIED Report.

16. Andersen, A.M., "Structural Studies of Metabolic Products of Dopamine, IV. Crystal 2nd Molecular Structure of (-) Noradrenaline," Acta Chem. Scand. Vol. 8, pp 871-876 (1975).

17. Byre, G., Arvid, M., and Romming, C., "Crystal and Molecular Structure of Clonidine Hydrochloride, 2-(2,6-D, Chlorophenylamino)-2-imidazoline Hydrochloride," Acta Chem. Scand. Vol. 9, pp 843-846 (1976).

18. Burket, U., and Allinger, N.L., Molecular Mechanics, ACS Monograph 177, American Chemical Society, Washington, DC, 1982.

19. Allinger, N.L., and Yuh, Y.H., "MM2," Quantum Chemistry Program Exchange (QCPE) Vol. 13, p 395 (1980).

20. Binkley, J.S., Whiteside, R.A., Raghavachari, K., Seeger, R., Defrees, D.J., Schlegel, H.B., Frisch, M.J., Pople, J.A., and Kahn, L.R., "GAUSSIAN82 RELEASE A," Carnegie-Mellon University, Pittsburgh, PA, 1982.

APPENDIX A

GEOMETRIC PARAMETER FILE FORMAT

The geometric parameter file contains the parameters required for implementing the Molecular Mechanics (MM2) computer program calculations in addition to those found in reference 14. The data records contained in the geometric parameter file are listed below.

Torsional dihedral angle parameters:

- 4 atom types comprising the torsional angle and v1, v2, and v3 values

ATOM TYPES				v1	v2	v3	Source and Date of Entry
1	1	8	18	0.00000	0.00000	0.30000	ash feb89
1	1	18	8	0.00000	0.00000	0.50000	ash feb89
1	3	2	9	0.00000	10.00000	0.50000	ash dec88
1	8	18	1	0.00000	0.00000	0.40000	ash feb89
1	8	18	7	0.00000	0.00000	0.40000	ash feb89
1	9	2	2	-0.40000	7.45000	0.00000	ash dec88
1	18	8	23	0.00000	0.00000	0.50000	ash feb89
2	3	1	9	0.00000	0.00000	-0.25000	ash dec88
2	9	1	3	0.00000	0.00000	-0.10000	ash dec88
5	1	8	18	0.00000	0.00000	0.30000	ash feb89
5	1	18	8	0.00000	0.00000	0.55000	ash feb89
5	15	18	6	0.00000	0.00000	0.50000	ash feb89
5	15	18	7	0.00000	0.00000	0.50000	ash feb89
6	1	1	18	-0.80000	0.00000	-0.30000	allinger feb89
7	18	8	23	0.00000	0.00000	0.40000	ash feb89
15	18	6	21	0.00000	0.00000	0.50000	ash feb89

Bond length parameters:

- 2 atom types comprising the atom bond lengths/stretches, the force constant (k), and the bond length (LO)

ATOM TYPES		k	LO	Source and Date of Entry
4	5	5.90000	1.09000	ash allinger feb89
4	10	17.73000	1.15800	ash allinger feb89
8	18	18.00000	1.70000	hopf feb89
15	18	5.00000	1.96000	ash feb89

Bond angle parameters:

- atom bond angles as defined by the three atom types, the angle force constant (k), and the atom bond length (A)

ATOM TYPE			k	A	Source and Date of Entry
1	8	18	0.50000	108.00000	ash feb89
1	18	8	0.60000	102.00000	ash feb89
5	15	18	0.48000	96.00000	ash feb89
6	18	15	0.56000	110.00000	ash feb89
7	18	8	0.80000	112.00000	ash feb89
7	18	15	0.75000	112.00000	ash feb89
18	8	23	0.45700	109.50000	ash feb89

APPENDIX B

COMPOUND STRUCTURE FILE FORMAT

The compound structure file is the primary data structure of Molecular Modeling, Analysis and Display System (MMADS) and it contains all the required molecular information. The data records contained in the chemical compound structure file are listed below.

Record #1 - the header record for the file

Column Nos. 1-3	the number of atoms contained in the file
Column Nos. 4-72	the title of the structure file

Record #2 - the descriptions of the individual atoms

Column Nos. 1	blank
Column Nos. 2-3	the atom symbol
Column Nos. 4-8	the atom index
Column Nos. 9-20	the x-coordinate
Column Nos. 21-32	the y-coordinate
Column Nos. 33-44	the z-coordinate
Column Nos. 45-49	the atom type (defined below)
Column Nos. 50-79	the atom bond connectivity

The MMADS uses the atom type to encode information describing each atom's molecular environment. The atom types used by MMADS are defined below.

Table. Atom Types Used by MMADS

Atom Type	Atom Type Description
1	Carbon - sp3
2	Carbon - sp2
3	Carbonyl Carbon
4	Carbon - sp
5	Hydrogen
6	Oxygen - sp3
7	Oxygen - sp2
8	Nitrogen - sp3
9	Nitrogen - sp2
10	Nitrogen - sp
11	Flourine
12	Chlorine
13	Bromine
14	Iodine

Table. Atom Types Used by MMADS (continued)

Atom Type	Atom Type Description
15	Sulfur - (-S-)
16	Sulfur - (=S)
17	Sulfur - (S oxide)
18	Sulfur - (SO2)
19	Silicon
20	(inactive)
21	Alcoholic Hydrogen (N-H, O-H)
22	Cyclopropane Hydrogen
23	Amine Hydrogen
24	Carboxyl Hydrogen
25	Phosphorus

33a2agon

N	1	-1.943300	-1.917320	-0.042390	9	5	2		
C	2	-2.564990	-3.161290	0.280210	1	1	3	16	33
C	3	-1.729480	-3.600370	1.490520	1	17	4	2	32
N	4	-1.380370	-2.359840	2.110930	8	18	5	3	
C	5	-1.238090	-1.433260	1.015480	2	12	4	1	
C	6	-0.518410	0.661280	-0.060180	2	12	11	7	
C	7	-1.300210	1.481900	-0.792700	2	19	8	6	
C	8	-0.807950	1.992480	-1.936240	2	20	9	7	
C	9	0.428420	1.694540	-2.359050	2	21	10	8	
C	10	1.203640	0.877260	-1.633880	2	13	11	9	
C	11	0.724040	0.366080	-0.489560	2	10	6	14	
C	12	-0.996310	0.040220	1.238700	1	22	15	6	5
H	13	2.223370	0.626850	-1.973490	5	10			
H	14	1.364190	-0.308780	0.104120	5	11			
H	15	-0.176320	0.114910	1.993090	5	12			
H	16	-2.503860	-3.876330	-0.572670	5	2			
H	17	-0.788670	-4.104330	1.162570	5	3			
H	18	-2.119140	-2.096300	2.757530	23	4			
C	19	-2.704500	1.857310	-0.367110	1	7	23	24	25
O	20	-1.550110	2.824150	-2.711520	6	8	30		
O	21	0.913980	2.212590	-3.515400	6	9	31		
C	22	-2.222030	0.758120	1.821230	1	12	23	26	27
C	23	-3.282440	0.968490	0.738890	1	19	22	28	29
H	24	-2.666110	2.911770	-0.004150	5	19			
H	25	-3.397330	1.830580	-1.241430	5	19			
H	26	-2.643120	0.189380	2.683920	5	22			
H	27	-1.916440	1.756850	2.216190	5	22			
H	28	-4.197330	1.440550	1.171750	5	23			
H	29	-3.601140	-0.013690	0.318880	5	23			
H	30	-1.979020	2.336880	-3.435530	21	20			
H	31	1.012290	3.178260	-3.457920	21	21			
H	32	-2.276370	-4.275780	2.190020	5	3			
H	33	-3.631470	-2.986140	0.556830	5	2			

29bht920

N	1	-2.430090	-1.783650	-0.756940	9	5	2		
C	2	-2.023820	-2.841100	-1.492650	2	13	3	1	
S	3	-0.273680	-2.890860	-1.689230	15	4	2		
C	4	-0.183850	-1.396760	-0.730710	2	5	3	12	
C	5	-1.400920	-0.981950	-0.336900	2	11	4	1	
C	6	1.356720	-0.242250	0.960500	1	12	7	14	15
N	7	0.543200	0.846570	1.421400	8	6	9	8	
C	8	-0.825110	0.497400	1.678190	1	11	7	16	17
C	9	0.711790	2.083890	0.701350	1	7	10	18	19
C	10	2.132110	2.590350	0.772490	2	9	20	21	
C	11	-1.715790	0.258010	0.452860	1	5	8	23	24
C	12	1.131490	-0.716390	-0.479900	1	4	6	25	26
N	13	-2.920190	-3.859390	-1.936940	8	2	27	28	
H	14	2.424170	0.060200	1.072610	5	6			
H	15	1.240180	-1.106360	1.656240	5	6			
H	16	-0.859590	-0.396420	2.344710	5	8			
H	17	-1.269820	1.320330	2.286800	5	8			
H	18	0.375800	1.984290	-0.355120	5	9			
H	19	0.078920	2.873340	1.169100	5	9			
C	20	2.892560	2.802460	-0.311320	2	10	22	29	
H	21	2.533040	2.781970	1.783040	5	10			
H	22	2.517490	2.615860	-1.330100	5	20			
H	23	-1.732570	1.131920	-0.237430	5	11			
H	24	-2.762580	0.153770	0.825850	5	11			
H	25	1.942890	-1.447700	-0.708130	5	12			
H	26	1.259390	0.104450	-1.221520	5	12			
H	27	-2.648450	-4.300810	-2.809750	23	13			
H	28	-3.866950	-3.533850	-2.104910	23	13			
H	29	3.927500	3.170680	-0.223760	5	20			

29bht9201n

S	1	-3.542250	-3.460310	-2.950540	15	5	2		
C	2	-2.565350	-4.796320	-2.341540	2	13	3	1	
N	3	-1.314960	-4.414060	-2.002130	9	4	2		
C	4	-1.100960	-3.070140	-2.155970	2	5	3	12	
C	5	-2.168100	-2.386980	-2.608590	2	11	4	1	
C	6	0.580720	-1.224840	-2.623350	1	12	7	14	15
N	7	-0.003940	-0.008230	-2.130680	8	6	9	8	
C	8	-1.408170	-0.099140	-1.823320	1	11	7	16	17
C	9	0.751300	0.598610	-1.055710	1	7	10	18	19
C	10	0.309190	2.017840	-0.789570	2	9	20	21	
C	11	-2.254850	-0.899910	-2.825010	1	5	8	23	24
C	12	0.249900	-2.492590	-1.824070	1	4	6	25	26
N	13	-2.973580	-6.163210	-2.307740	8	2	27	28	
H	14	0.274570	-1.363190	-3.686260	5	6			
H	15	1.687500	-1.098720	-2.683010	5	6			
H	16	-1.565160	-0.518730	-0.800770	5	8			
H	17	-1.805930	0.942880	-1.808390	5	8			
H	18	0.696000	-0.028540	-0.135380	5	9			
H	19	1.826420	0.671040	-1.340900	5	9			
C	20	-0.170540	2.430970	0.392280	2	10	22	29	
H	21	0.395530	2.723010	-1.634590	5	10			
H	22	-0.270490	1.746490	1.249540	5	20			
H	23	-2.013540	-0.642650	-3.882560	5	11			
H	24	-3.319930	-0.607910	-2.663840	5	11			
H	25	0.337150	-2.336610	-0.724300	5	12			
H	26	1.004310	-3.267680	-2.098770	5	12			
H	27	-2.870770	-6.644990	-3.195180	23	13			
H	28	-3.945590	-6.302780	-2.051150	23	13			
H	29	-0.486960	3.474570	0.551000	5	20			

28bht9331n

O	1	-3.147481	-3.442131	-2.940331	6	5	2	0	0	0	0
C	2	-2.619441	-4.580950	-2.421250	2	13	3	1	0	0	0
N	3	-1.355101	-4.472810	-1.968900	9	4	2	0	0	0	0
C	4	-1.083790	-3.155741	-2.140640	2	5	3	12	0	0	0
C	5	-2.150521	-2.544441	-2.679550	2	11	4	1	0	0	0
C	6	0.546410	-1.273840	-2.587630	1	12	7	14	15	0	0
N	7	-0.116720	-0.065730	-2.172380	8	6	9	8	0	0	0
C	8	-1.538100	-0.192140	-1.979660	1	11	7	16	17	0	0
C	9	0.549560	0.590760	-1.064210	1	7	10	18	19	0	0
C	10	-0.020500	1.973610	-0.711340	1	9	20	21	28	0	0
C	11	-2.282821	-1.081050	-2.988481	1	5	8	22	23	0	0
C	12	0.229530	-2.531370	-1.765970	1	4	6	24	25	0	0
N	13	-3.241671	-5.863001	-2.509700	8	2	26	27	0	0	0
H	14	0.311330	-1.458920	-3.661460	5	6	0	0	0	0	0
H	15	1.648510	-1.100900	-2.587280	5	6	0	0	0	0	0
H	16	-1.763140	-0.552460	-0.947270	5	8	0	0	0	0	0
H	17	-1.969410	0.831360	-2.076470	5	8	0	0	0	0	0
H	18	0.530540	-0.059500	-0.157679	5	9	0	0	0	0	0
H	19	1.619730	0.749360	-1.337320	5	9	0	0	0	0	0
H	20	0.637001	2.496441	0.021811	5	10	0	0	0	0	0
H	21	-1.027590	1.909041	-0.239349	5	10	0	0	0	0	0
H	22	-1.983261	-0.873220	-4.041840	5	11	0	0	0	0	0
H	23	-3.371231	-0.846320	-2.913760	5	11	0	0	0	0	0
H	24	0.260260	-2.343680	-0.668360	5	12	0	0	0	0	0
H	25	1.016690	-3.290690	-1.986990	5	12	0	0	0	0	0
H	26	-3.084862	-6.334301	-3.394911	23	13	0	0	0	0	0
H	27	-4.251421	-5.838822	-2.409460	23	13	0	0	0	0	0
H	28	-0.094550	2.620760	-1.615870	5	10	0	0	0	0	0

45ch-38038

C	1	2.852725	0.427810	0.180884	2	23	6	2	0	0	0
C	2	4.046250	0.515862	0.780051	2	9	3	1	0	0	0
C	3	4.143273	0.654469	2.107598	2	7	4	2	0	0	0
C	4	3.045404	0.705230	2.868885	2	24	5	3	0	0	0
C	5	1.840942	0.614077	2.275928	2	10	6	4	0	0	0
C	6	1.739393	0.480904	0.936475	2	13	5	1	0	0	0
O	7	5.441426	0.732997	2.491831	6	8	3	0	0	0	0
C	8	6.113196	0.275387	1.338142	1	26	25	9	7	0	0
O	9	5.281088	0.492267	0.218474	6	8	2	0	0	0	0
C	10	0.570585	0.674501	3.097542	1	28	27	11	5	0	0
C	11	-0.576740	-0.184735	2.528032	1	30	29	12	10	0	0
N	12	-0.353091	-0.604742	1.175070	8	14	13	11	0	0	0
C	13	0.327739	0.386975	0.393060	1	31	17	12	6	0	0
C	14	-1.457721	-1.263895	0.541847	1	33	32	15	12	0	0
C	15	-2.240520	-0.334594	-0.395058	1	34	18	16	14	0	0
C	16	-1.315068	0.207704	-1.508496	1	35	21	17	15	0	0
C	17	0.172628	0.100921	-1.108896	1	37	36	16	13	0	0
C	18	-3.493375	-1.029143	-0.960368	1	39	38	19	15	0	0
C	19	-4.038139	-0.239512	-2.156131	1	41	40	20	18	0	0
C	20	-3.037167	-0.260777	-3.322767	1	42	22	21	19	0	0
C	21	-1.585798	-0.470670	-2.859803	1	44	43	20	16	0	0
O	22	-3.118173	0.967272	-4.015456	6	45	20	0	0	0	0
H	23	2.807925	0.313741	-0.912627	5	1	0	0	0	0	0
H	24	3.136869	0.822920	3.961044	5	4	0	0	0	0	0
H	25	7.056201	0.854558	1.210306	5	8	0	0	0	0	0
H	26	6.312021	-0.818595	1.439890	5	8	0	0	0	0	0
H	27	0.261628	1.746695	3.119500	5	10	0	0	0	0	0
H	28	0.764314	0.382753	4.157007	5	10	0	0	0	0	0
H	29	-1.537426	0.379362	2.604217	5	11	0	0	0	0	0
H	30	-0.681214	-1.108970	3.144361	5	11	0	0	0	0	0
H	31	-0.151606	1.383064	0.557356	5	13	0	0	0	0	0
H	32	-2.130265	-1.726462	1.301924	5	14	0	0	0	0	0
H	33	-1.048848	-2.115067	-0.049992	5	14	0	0	0	0	0
H	34	-2.589851	0.532173	0.219668	5	15	0	0	0	0	0
H	35	-1.552733	1.292249	-1.644708	5	16	0	0	0	0	0
H	36	0.576269	-0.912859	-1.339858	5	17	0	0	0	0	0
H	37	0.748438	0.834433	-1.721733	5	17	0	0	0	0	0
H	38	-3.256785	-2.068790	-1.287504	5	18	0	0	0	0	0
H	39	-4.270461	-1.114866	-0.163223	5	18	0	0	0	0	0
H	40	-4.227617	0.809686	-1.826856	5	19	0	0	0	0	0
H	41	-5.019613	-0.654351	-2.488910	5	19	0	0	0	0	0
H	42	-3.300385	-1.055300	-4.063041	5	20	0	0	0	0	0
H	43	-1.380447	-1.562147	-2.754355	5	21	0	0	0	0	0
H	44	-0.880570	-0.092674	-3.637677	5	21	0	0	0	0	0
H	45	-3.994707	1.030137	-4.431637	21	22	0	0	0	0	0

23 clonidine crystal structure---Byre 1976

CL	1	1.563190	-0.105335	3.731911	12	7	0	0	0	0	0
CL	2	5.460859	0.320600	5.683131	12	11	0	0	0	0	0
N	3	2.684705	1.475205	3.337569	9	6	12	0	0	0	0
N	4	2.646133	0.065349	1.447837	8	12	13	19	0	0	0
N	5	1.388007	2.860291	0.398715	8	12	14	23	0	0	0
C	6	3.602281	-0.030904	4.827628	2	3	7	11	0	0	0
C	7	3.205207	-0.877161	5.160756	2	1	6	8	0	0	0
C	8	4.093329	-2.330804	6.624854	2	7	9	15	0	0	0
C	9	5.402932	-2.967619	7.788754	2	8	10	20	0	0	0
C	10	5.823429	-2.154309	7.506865	2	9	11	16	0	0	0
C	11	4.929276	-0.697517	6.037438	2	2	6	10	0	0	0
C	12	2.269677	1.455662	1.794356	2	3	4	5	0	0	0
C	13	1.963491	0.513085	-0.373847	1	4	14	17	21	0	0
C	14	1.072003	2.472156	-1.112386	1	5	13	18	22	0	0
H	15	3.801029	-2.871369	6.777344	5	8	0	0	0	0	0
H	16	6.676346	-2.517094	8.239391	5	10	0	0	0	0	0
H	17	2.552721	0.038570	-0.669536	5	13	0	0	0	0	0
H	18	0.098182	2.968760	-1.912960	5	14	0	0	0	0	0
H	19	3.310121	-0.901521	2.227232	23	4	0	0	0	0	0
H	20	5.589383	-3.809853	8.438582	5	9	0	0	0	0	0
H	21	1.514802	0.067668	-0.792512	5	13	0	0	0	0	0
H	22	1.248309	2.861911	-1.735328	5	14	0	0	0	0	0
H	23	1.009868	3.805378	0.368928	23	5	0	0	0	0	0

26flutonidine

N	1	-2.221670	-1.794120	0.236740	8	5	2	22	
C	2	-3.352020	-2.645540	0.438610	1	3	1	16	23
C	3	-2.808050	-3.699070	1.411590	1	4	2	15	17
N	4	-1.939860	-2.942640	2.264120	8	18	5	3	
C	5	-1.449820	-1.867380	1.446760	2	12	4	1	
C	6	0.429540	-0.860580	2.711580	2	12	11	7	
C	7	0.456890	-1.649970	3.799670	2	19	8	6	
C	8	1.362470	-1.425050	4.765400	2	20	9	7	
C	9	2.241160	-0.418040	4.652620	2	21	10	8	
C	10	2.210630	0.366870	3.564240	2	13	11	9	
C	11	1.308610	0.153080	2.588350	2	10	6	14	
N	12	-0.446470	-1.013140	1.690540	9	6	5		
H	13	2.936320	1.193210	3.477390	5	10			
C	14	1.286530	1.047180	1.367230	1	11	24	25	26
H	15	-3.604010	-4.218070	1.996250	5	3			
H	16	-4.182790	-2.066480	0.910060	5	2			
H	17	-2.197700	-4.461290	0.870800	5	3			
H	18	-2.462010	-2.610040	3.070570	23	4			
H	19	-0.250270	-2.484800	3.918060	5	7			
F	20	1.387070	-2.148370	5.761280	11	8			
H	21	2.985200	-0.234320	5.447300	5	9			
H	22	-2.512170	-0.859680	-0.033090	23	1			
H	23	-3.695780	-3.075330	-0.531000	5	2			
H	24	1.478110	0.454380	0.443540	5	14			
H	25	0.299930	1.555550	1.269570	5	14			
H	26	2.060380	1.847230	1.405610	5	14			

22guanabenz

N	1	-2.237940	-2.090590	0.959460	8	5	2	21
C	2	-3.021690	-1.062980	0.315680	2	1	3	15
N	3	-2.304240	-0.450110	-0.664640	9	2	4	
H	4	-1.971750	-1.047790	-1.409180	23	3		
N	5	-1.433380	-1.756650	1.785740	9	12	1	
C	6	0.716870	-0.966410	2.432690	2	12	11	7
C	7	1.965590	-0.611740	2.035680	2	18	8	6
C	8	2.878870	-0.201020	2.933860	2	19	9	7
C	9	2.574850	-0.133170	4.235030	2	20	10	8
C	10	1.346160	-0.480880	4.635470	2	13	11	9
C	11	0.415720	-0.895760	3.754920	2	10	6	14
C	12	-0.171920	-1.371210	1.495660	2	6	5	22
H	13	1.109240	-0.419460	5.712310	5	10		
CL	14	-1.158980	-1.307670	4.503390	12	11		
N	15	-4.179670	-1.714390	-0.245260	8	2	16	17
H	16	-4.837030	-1.081070	-0.689540	23	15		
H	17	-3.976650	-2.412040	-0.954710	23	15		
CL	18	2.528440	-0.647780	0.335600	12	7		
H	19	3.894260	0.086820	2.609440	5	8		
H	20	3.327800	0.205080	4.968280	5	9		
H	21	-1.982160	-2.873620	0.364860	23	1		
H	22	0.078640	-1.421810	0.424050	5	12		

31guanacline

N	1	1.408130	3.165460	-0.843450	8	5	2	21	
C	2	0.467410	3.850840	-1.680270	2	1	3	15	
N	3	0.823800	4.245890	-2.916460	9	2	4		
H	4	1.800580	4.133910	-3.149500	23	3			
C	5	1.698220	1.795030	-1.117320	1	12	1	30	31
N	6	-0.058350	0.938320	0.463590	8	12	11	7	
C	7	-1.278730	0.182350	0.579670	1	18	8	6	23
C	8	-1.989820	0.491580	1.903650	1	19	9	7	24
C	9	-1.040050	0.410920	3.066010	2	20	10	8	
C	10	0.283750	0.443950	2.856480	2	13	11	9	
C	11	0.893040	0.558220	1.481920	1	10	6	14	25
C	12	0.492480	0.869140	-0.875710	1	6	5	22	29
H	13	0.990940	0.381610	3.701090	5	10			
H	14	1.372960	-0.418300	1.235700	5	11			
N	15	-0.921900	3.835550	-1.336760	8	2	16	17	
H	16	-1.103510	3.811650	-0.338260	23	15			
H	17	-1.441370	4.642090	-1.668410	23	15			
H	18	-1.978260	0.443370	-0.249770	5	7			
H	19	-2.824420	-0.234150	2.049430	5	8			
C	20	-1.643370	0.328260	4.444540	1	9	26	27	28
H	21	1.248740	3.303840	0.149710	23	1			
H	22	0.781600	-0.183100	-1.112490	5	12			
H	23	-1.056650	-0.909580	0.501880	5	7			
H	24	-2.425660	1.518270	1.884580	5	8			
H	25	1.680900	1.342060	1.546400	5	11			
H	26	-2.292370	1.213820	4.630240	5	20			
H	27	-2.264750	-0.591030	4.537580	5	20			
H	28	-0.871280	0.298030	5.246520	5	20			
H	29	-0.298090	1.152520	-1.609340	5	12			
H	30	2.030330	1.709570	-2.179200	5	5			
H	31	2.577810	1.488050	-0.506130	5	5			

34guanadrel

C	1	0.794080	3.251270	1.338620	1	17	16	6	2
C	2	-0.382870	2.738980	0.496130	1	19	18	3	1
C	3	-0.514650	1.213770	0.610630	1	21	20	4	2
C	4	0.791150	0.507730	0.222180	1	10	7	5	3
C	5	1.976750	1.035400	1.041150	1	23	22	6	4
C	6	2.102280	2.561370	0.926350	1	25	24	5	1
O	7	1.053220	0.717670	-1.155500	6	8	4		
C	8	0.796670	-0.511570	-1.793810	1	27	26	9	7
C	9	1.105640	-1.527230	-0.702110	1	28	11	10	8
O	10	0.640000	-0.881250	0.461260	6	9	4		
C	11	0.399610	-2.874380	-0.870620	1	30	29	12	9
N	12	0.656110	-3.736090	0.235940	8	31	13	11	
C	13	0.020040	-5.009940	0.390770	3	15	14	12	
N	14	-1.241030	-4.926850	1.059590	8	33	32	13	
N	15	0.471930	-6.088680	-0.129570	9	34	13		
H	16	0.593040	3.053460	2.418490	5	1			
H	17	0.893540	4.357190	1.220450	5	1			
H	18	-0.227930	3.022640	-0.571980	5	2			
H	19	-1.329980	3.227960	0.829010	5	2			
H	20	-1.349780	0.852100	-0.035300	5	3			
H	21	-0.775970	0.946680	1.661950	5	3			
H	22	2.921880	0.549100	0.701040	5	5			
H	23	1.833120	0.758290	2.112320	5	5			
H	24	2.354410	2.839160	-0.124640	5	6			
H	25	2.941190	2.922540	1.568790	5	6			
H	26	1.454770	-0.594710	-2.689000	5	8			
H	27	-0.277820	-0.511630	-2.091980	5	8			
H	28	2.209150	-1.657520	-0.583180	5	9			
H	29	0.749220	-3.368730	-1.807280	5	11			
H	30	-0.701280	-2.716150	-0.948200	5	11			
H	31	1.655180	-3.783010	0.414910	23	12			
H	32	-1.466460	-5.750870	1.607580	23	14			
H	33	-2.023940	-4.820710	0.422250	23	14			
H	34	0.134780	-6.162310	-1.080090	23	15			

24guanfacine

N	1	-1.905360	-2.169550	0.179750	8	5	2	21	
C	2	-2.376350	-1.680950	-1.100560	2	1	3	15	
N	3	-1.342770	-1.748950	-1.983390	9	2	4		
H	4	-0.928140	-2.659910	-2.125600	23	3			
C	5	-1.033760	-1.401220	1.029170	3	12	1	24	
C	6	0.962990	-1.280340	2.557170	2	12	11	7	
C	7	2.043440	-0.627020	2.074650	2	18	8	6	
C	8	2.772210	0.157770	2.888090	2	19	9	7	
C	9	2.437150	0.303250	4.177310	2	20	10	8	
C	10	1.362680	-0.338270	4.656380	2	13	11	9	
C	11	0.623270	-1.126910	3.856510	2	10	6	14	
C	12	0.124780	-2.169520	1.646900	1	6	5	22	23
H	13	1.090080	-0.209210	5.718310	5	10			
CL	14	-0.797310	-1.931420	4.580960	12	11			
N	15	-3.431400	-2.575470	-1.513120	8	2	16	17	
H	16	-3.862520	-2.326260	-2.397820	23	15			
H	17	-3.153700	-3.545490	-1.628140	23	15			
CL	18	2.563490	-0.746070	0.370270	12	7			
H	19	3.655810	0.694060	2.500350	5	8			
H	20	3.039440	0.950050	4.838900	5	9			
H	21	-1.643080	-3.151890	0.152620	23	1			
H	22	-0.274880	-3.049960	2.198520	5	12			
H	23	0.730410	-2.618050	0.828130	5	12			
O	24	-1.232620	-0.229230	1.252850	7	5			

36imiloxan-rs21361

C	1	-3.251610	-0.942640	2.005700	2	17	6	2	
C	2	-3.443840	-0.137590	3.063410	2	18	3	1	
C	3	-2.579200	0.858180	3.318210	2	19	4	2	
C	4	-1.519110	1.051460	2.516600	2	20	5	3	
C	5	-1.325000	0.243890	1.461100	2	7	6	4	
C	6	-2.193600	-0.746280	1.202070	2	10	5	1	
O	7	-0.239070	0.520790	0.687880	6	8	5		
C	8	0.093330	-0.577000	-0.138990	1	7	9	11	29
C	9	-1.188610	-1.076770	-0.815200	1	22	21	10	8
O	10	-2.051360	-1.615200	0.162960	6	9	6		
H	11	0.771790	-0.149450	-0.915730	5	8			
C	12	1.299800	-2.798930	-0.194420	2	13	16	29	
N	13	2.002260	-2.537030	-1.333180	9	14	12		
C	14	3.031260	-3.503330	-1.558490	1	26	25	15	13
C	15	2.535960	-4.668870	-0.689700	1	28	27	16	14
N	16	1.911890	-3.966390	0.390210	8	12	15	23	
H	17	-3.960940	-1.763110	1.801100	5	1			
H	18	-4.313160	-0.295420	3.725150	5	2			
H	19	-2.740550	1.519200	4.187440	5	3			
H	20	-0.812400	1.872910	2.726460	5	4			
H	21	-1.730490	-0.264940	-1.357460	5	9			
H	22	-0.977240	-1.899660	-1.536000	5	9			
C	23	1.193600	-4.778570	1.322250	1	16	24	32	33
C	24	-0.138000	-5.323820	0.787070	1	23	34	35	36
H	25	4.007280	-3.102320	-1.196120	5	14			
H	26	3.106170	-3.767350	-2.638940	5	14			
H	27	1.789940	-5.275450	-1.256200	5	15			
H	28	3.365580	-5.323440	-0.333060	5	15			
C	29	0.858310	-1.642330	0.666430	1	8	12	30	31
H	30	0.221640	-2.036580	1.489920	5	29			
H	31	1.761000	-1.184300	1.134650	5	29			
H	32	1.846750	-5.618690	1.657040	5	23			
H	33	0.995460	-4.163030	2.230580	5	23			
H	34	0.006930	-6.035530	-0.056890	5	24			
H	35	-0.685270	-5.874940	1.586600	5	24			
H	36	-0.803990	-4.502230	0.435500	5	24			

491654284

C	1	-3.199740	0.793250	-5.761820	2	27	6	2	
C	2	-4.414480	0.378290	-6.162530	2	28	3	1	
C	3	-5.116640	-0.504390	-5.427500	2	4	2	48	
C	4	-4.618410	-0.990580	-4.276610	2	5	3	49	
C	5	-3.408260	-0.568420	-3.888320	2	7	6	4	
C	6	-2.705650	0.310290	-4.616170	2	9	5	1	
C	7	-2.686280	-0.878000	-2.808280	2	10	8	5	
C	8	-1.542740	-0.186570	-2.863980	2	13	9	7	
O	9	-1.516570	0.567960	-4.001000	6	8	6		
C	10	-2.994350	-1.814150	-1.683340	1	30	29	11	7
C	11	-1.672000	-2.219130	-1.009070	1	32	31	12	10
N	12	-0.872620	-1.064060	-0.679730	8	14	13	11	
C	13	-0.469860	-0.273350	-1.816890	1	33	17	12	8
C	14	0.250450	-1.387890	0.170320	1	35	34	15	12
C	15	1.245330	-0.218850	0.322050	1	36	18	16	14
C	16	0.519710	1.116160	0.090800	1	37	21	17	15
C	17	-0.069560	1.137290	-1.336510	1	39	38	16	13
H	18	1.727910	-0.262790	1.326700	5	15			
C	19	1.257940	2.567130	1.857080	1	21	20	22	23
H	20	1.838110	1.796580	2.415420	5	19			
N	21	1.258590	2.324680	0.432230	8	16	19	24	
H	22	1.663360	3.573150	2.102770	5	19			
H	23	0.216620	2.582820	2.251970	5	19			
S	24	2.805050	2.506050	-0.260170	18	21	25	26	40
O	25	3.770580	1.748380	0.364130	7	24			
O	26	2.852730	2.213200	-1.604420	7	24			
H	27	-2.619340	1.515850	-6.359570	5	1			
H	28	-4.839690	0.766020	-7.104500	5	2			
H	29	-3.529730	-2.718370	-2.057060	5	10			
H	30	-3.655030	-1.285530	-0.956610	5	10			
H	31	-1.092330	-2.896880	-1.681400	5	11			
H	32	-1.913900	-2.788210	-0.080100	5	11			
H	33	0.398240	-0.771660	-2.312760	5	13			
H	34	-0.160540	-1.648600	1.174220	5	14			
H	35	0.793810	-2.284730	-0.213780	5	14			
H	36	2.058990	-0.331470	-0.432570	5	15			
H	37	-0.376440	1.081630	0.757430	5	16			
H	38	-0.964550	1.805080	-1.328050	5	17			
H	39	0.623170	1.578070	-2.087090	5	17			
C	40	3.228900	4.272240	-0.082270	1	24	41	44	45
C	41	4.567520	4.627460	-0.740650	1	40	42	46	47
O	42	4.816970	5.999170	-0.532080	6	41	43		
H	43	5.665360	6.228420	-0.947990	21	42			
H	44	2.409940	4.871590	-0.544040	5	40			
H	45	3.285170	4.531840	0.999080	5	40			
H	46	5.417090	4.065910	-0.285650	5	41			
H	47	4.547720	4.460210	-1.843190	5	41			
H	48	-6.112340	-0.833180	-5.772390	5	3			
H	49	-5.192730	-1.712800	-3.672170	5	4			

26methnor1r2r- amethylnoradrenaline 1R,2R (n3)											
O	1	-1.774173	2.936789	-1.335066	6	7	23	0	0	0	0
O	2	0.649462	4.123841	-0.782302	6	8	21	0	0	0	0
O	3	1.182687	-2.017031	-1.192623	6	11	22	0	0	0	0
N	4	-0.016072	-3.355225	0.960802	8	12	19	20	0	0	0
C	5	0.240935	0.095729	-0.573760	2	6	10	11	0	0	0
C	6	-0.817306	0.853147	-0.917095	2	5	7	13	0	0	0
C	7	-0.696764	2.188007	-0.987118	2	1	6	8	0	0	0
C	8	0.475551	2.779017	-0.715786	2	2	7	9	0	0	0
C	9	1.536064	2.031432	-0.373614	2	8	10	14	0	0	0
C	10	1.414637	0.695806	-0.302235	2	5	9	15	0	0	0
C	11	0.117441	-1.412979	-0.490999	1	3	5	12	16	0	0
C	12	0.120068	-1.931177	0.959063	1	4	11	17	18	0	0
H	13	-1.788897	0.381848	-1.141060	5	6	0	0	0	0	0
H	14	2.505262	2.510433	-0.151347	5	9	0	0	0	0	0
H	15	2.290896	0.088758	-0.018459	5	10	0	0	0	0	0
H	16	-0.808734	-1.763601	-1.005246	5	11	0	0	0	0	0
C	17	-1.026218	-1.320939	1.782167	1	12	24	25	26	0	0
H	18	1.091708	-1.673406	1.447097	5	12	0	0	0	0	0
H	19	0.003915	-3.715995	1.909761	23	4	0	0	0	0	0
H	20	0.778720	-3.796252	0.508741	23	4	0	0	0	0	0
H	21	-0.188002	4.615756	-0.785972	21	2	0	0	0	0	0
H	22	1.194427	-1.669667	-2.100657	21	3	0	0	0	0	0
H	23	-2.504342	2.836286	-0.700650	21	1	0	0	0	0	0
H	24	-1.037404	-1.721983	2.822049	5	17	0	0	0	0	0
H	25	-0.928334	-0.214234	1.863674	5	17	0	0	0	0	0
H	26	-2.015527	-1.544311	1.320631	5	17	0	0	0	0	0

26	amethnor1R2S-amethylnoradrenaline-1R,2S(-)			ch3	extended		(n5)				
O	1	-3.400830	1.461850	-1.068570	6	7	23	0	0	0	0
O	2	-1.892910	3.752800	-0.811110	6	8	21	0	0	0	0
O	3	1.748970	-1.236480	-1.279830	6	11	22	0	0	0	0
N	4	-0.354010	-1.615650	1.673590	8	12	19	20	0	0	0
C	5	-0.134190	0.105190	-0.621060	2	6	10	11	0	0	0
C	6	-1.463500	0.191890	-0.812700	2	5	7	13	0	0	0
C	7	-2.059050	1.392990	-0.874970	2	1	6	8	0	0	0
C	8	-1.337660	2.515600	-0.746140	2	2	7	9	0	0	0
C	9	-0.011700	2.438410	-0.554920	2	8	10	14	0	0	0
C	10	0.583640	1.236200	-0.490750	2	5	9	15	0	0	0
C	11	0.544550	-1.248570	-0.544930	1	3	5	12	16	0	0
C	12	0.851510	-1.649740	0.908580	1	4	11	17	18	0	0
H	13	-2.070460	-0.722990	-0.917630	5	6	0	0	0	0	0
H	14	0.589010	3.358330	-0.449550	5	9	0	0	0	0	0
H	15	1.673500	1.182100	-0.329020	5	10	0	0	0	0	0
H	16	-0.085620	-2.033260	-1.026900	5	11	0	0	0	0	0
H	17	1.548400	-0.898590	1.352950	5	12	0	0	0	0	0
C	18	1.498980	-3.041150	0.999620	1	12	24	25	26	0	0
H	19	-0.177370	-1.871270	2.639960	23	4	0	0	0	0	0
H	20	-1.011690	-2.312540	1.338700	23	4	0	0	0	0	0
H	21	-2.857690	3.742860	-0.699580	21	2	0	0	0	0	0
H	22	1.555410	-0.953110	-2.189530	21	3	0	0	0	0	0
H	23	-3.892550	1.031960	-0.348070	21	1	0	0	0	0	0
H	24	1.708380	-3.321380	2.057890	5	18	0	0	0	0	0
H	25	0.836950	-3.825580	0.566090	5	18	0	0	0	0	0
H	26	2.468720	-3.073670	0.452110	5	18	0	0	0	0	0

26amethnor1R2SNH2-amethylnoradrenaline-1R,2S (-) nh2 extended (n4)

O	1	-3.436161	1.418226	-0.704066	6	7	23	0	0	0	0
O	2	-1.945815	3.734386	-0.715568	6	8	21	0	0	0	0
O	3	1.842996	-1.184808	-1.202647	6	11	22	0	0	0	0
N	4	1.230245	-3.121621	0.778208	8	12	19	20	0	0	0
C	5	-0.116175	0.115824	-0.625773	2	6	10	11	0	0	0
C	6	-1.460392	0.181425	-0.649730	2	5	7	13	0	0	0
C	7	-2.079804	1.371653	-0.677673	2	1	6	8	0	0	0
C	8	-1.366940	2.506896	-0.679331	2	2	7	9	0	0	0
C	9	-0.026500	2.452061	-0.655439	2	8	10	14	0	0	0
C	10	0.592465	1.260452	-0.627702	2	5	9	15	0	0	0
C	11	0.571812	-1.235386	-0.592927	1	3	5	12	16	0	0
C	12	0.717985	-1.788728	0.836471	1	4	11	17	18	0	0
H	13	-2.059532	-0.744648	-0.645932	5	6	0	0	0	0	0
H	14	0.567346	3.382419	-0.658346	5	9	0	0	0	0	0
H	15	1.694675	1.230499	-0.603907	5	10	0	0	0	0	0
H	16	-0.012686	-1.958512	-1.211299	5	11	0	0	0	0	0
H	17	-0.300514	-1.855710	1.290804	5	12	0	0	0	0	0
C	18	1.601169	-0.915406	1.741635	1	12	24	25	26	0	0
H	19	1.274501	-3.532003	1.705807	23	4	0	0	0	0	0
H	20	2.191504	-3.124995	0.452377	23	4	0	0	0	0	0
H	21	-2.888950	3.716830	-0.484197	21	2	0	0	0	0	0
H	22	1.741339	-0.852358	-2.110661	21	3	0	0	0	0	0
H	23	-3.827713	1.001941	0.082762	21	1	0	0	0	0	0
H	24	1.709493	-1.366239	2.755126	5	18	0	0	0	0	0
H	25	2.623701	-0.790321	1.317746	5	18	0	0	0	0	0
H	26	1.161952	0.098119	1.884263	5	18	0	0	0	0	0

26Amethnor1s2r- amethylnoradrenaline 1S,2R (n6)

O	1	-1.765720	2.922980	-1.297220	6	7	23	0	0	0	0
O	2	0.626730	4.136110	-0.830020	6	8	21	0	0	0	0
H	3	1.131790	-1.851430	-0.933080	5	11	0	0	0	0	0
N	4	0.054110	-3.322200	1.010700	8	12	19	20	0	0	0
C	5	0.300410	0.103190	-0.572540	2	6	10	11	0	0	0
C	6	-0.777240	0.845030	-0.889770	2	5	7	13	0	0	0
C	7	-0.676380	2.180690	-0.973310	2	1	6	8	0	0	0
C	8	0.495640	2.788270	-0.741630	2	2	7	9	0	0	0
C	9	1.575620	2.059020	-0.423860	2	8	10	14	0	0	0
C	10	1.472870	0.722620	-0.339320	2	5	9	15	0	0	0
C	11	0.218830	-1.407800	-0.467550	1	3	5	12	16	0	0
C	12	0.092080	-1.892880	0.988350	1	4	11	17	18	0	0
H	13	-1.750990	0.364690	-1.080220	5	6	0	0	0	0	0
H	14	2.543770	2.553420	-0.233370	5	9	0	0	0	0	0
H	15	2.364570	0.128760	-0.075600	5	10	0	0	0	0	0
O	16	-0.859180	-1.928540	-1.213850	6	11	22	0	0	0	0
C	17	-1.158590	-1.341630	1.690910	1	12	24	25	26	0	0
H	18	0.994890	-1.564540	1.560060	5	12	0	0	0	0	0
H	19	0.038540	-3.666330	1.965840	23	4	0	0	0	0	0
H	20	0.905420	-3.710250	0.616130	23	4	0	0	0	0	0
H	21	-0.100400	4.604820	-0.387070	21	2	0	0	0	0	0
H	22	-0.749290	-1.668140	-2.144240	21	16	0	0	0	0	0
H	23	-2.515570	2.748490	-0.702930	21	1	0	0	0	0	0
H	24	-1.239780	-1.728030	2.733220	5	17	0	0	0	0	0
H	25	-1.132790	-0.230140	1.759640	5	17	0	0	0	0	0
H	26	-2.088920	-1.631270	1.150820	5	17	0	0	0	0	0

26amethnor1S2S-amethylnoradrenaline 1S,2S (n7)

O	1	-1.810720	2.941740	-0.999240	6	7	23		
O	2	0.629120	4.137520	-0.830490	6	8	21		
H	3	1.205940	-1.881880	-0.747100	5	11			
N	4	-0.444730	-3.312360	0.801650	8	12	19	20	
C	5	0.320740	0.103090	-0.617800	2	6	10	11	
C	6	-0.786610	0.852250	-0.771130	2	5	7	13	
C	7	-0.692450	2.189210	-0.838840	2	1	6	8	
C	8	0.503650	2.788390	-0.754120	2	2	7	9	
C	9	1.613530	2.050580	-0.601450	2	8	10	14	
C	10	1.518060	0.712680	-0.532960	2	5	9	15	
C	11	0.217860	-1.407160	-0.538020	1	3	5	12	16
C	12	-0.308950	-1.890130	0.825020	1	4	11	17	18
H	13	-1.776520	0.371420	-0.841400	5	6			
H	14	2.600610	2.539460	-0.533010	5	9			
H	15	2.435100	0.113050	-0.404380	5	10			
O	16	-0.644670	-1.887640	-1.546560	6	11	22		
H	17	-1.328170	-1.465450	0.992540	5	12			
C	18	0.605200	-1.464070	1.985180	1	12	24	25	26
H	19	-0.815500	-3.654730	1.682540	23	4			
H	20	0.462960	-3.758450	0.714780	23	4			
H	21	-0.039610	4.598810	-0.297010	21	2			
H	22	-0.323980	-1.568650	-2.407280	21	16			
H	23	-2.491950	2.729920	-0.338310	21	1			
H	24	0.233450	-1.858090	2.959180	5	18			
H	25	1.643970	-1.840140	1.840200	5	18			
H	26	0.653550	-0.355150	2.079700	5	18			

34midagaa

C	1	3.755000	1.579570	0.582050	2	21	6	2	
C	2	3.997760	0.258640	0.516740	2	7	3	1	
C	3	3.112600	-0.537440	-0.109840	2	22	4	2	
C	4	2.000220	-0.017060	-0.656520	2	15	5	3	
C	5	1.758140	1.301230	-0.584320	2	8	6	4	
C	6	2.645070	2.099630	0.033040	2	23	5	1	
CL	7	5.473160	-0.425460	1.245510	12	2			
O	8	0.651980	1.882370	-1.124110	6	9	5		
C	9	-0.469290	1.834890	-0.353110	2	14	10	8	
C	10	-1.500680	1.099910	-0.801190	2	24	11	9	
C	11	-2.631900	1.023410	-0.081750	2	25	12	10	
C	12	-2.734780	1.686360	1.081360	2	26	13	11	
C	13	-1.706700	2.427980	1.524010	2	27	14	12	
C	14	-0.573970	2.503900	0.806820	2	28	13	9	
N	15	1.127310	-0.838540	-1.283060	9	16	4		
C	16	0.315010	-1.612290	-0.667010	3	20	17	15	
N	17	-0.627710	-2.508180	-1.274620	8	29	18	16	
C	18	-1.154140	-3.383130	-0.264230	1	31	30	19	17
C	19	-1.022020	-2.540510	1.015980	1	33	32	20	18
N	20	0.157260	-1.771410	0.750190	8	34	19	16	
H	21	4.472340	2.248540	1.088070	5	1			
H	22	3.300430	-1.623190	-0.175180	5	3			
H	23	2.466470	3.187130	0.090500	5	6			
H	24	-1.422100	0.558970	-1.759640	5	10			
H	25	-3.477760	0.416060	-0.447910	5	11			
H	26	-3.665340	1.623980	1.671770	5	12			
H	27	-1.793180	2.976320	2.478150	5	13			
H	28	0.263080	3.119100	1.175930	5	14			
H	29	-1.387820	-2.003910	-1.723090	23	17			
H	30	-2.201520	-3.692790	-0.491510	5	18			
H	31	-0.502450	-4.287210	-0.209730	5	18			
H	32	-0.895180	-3.149530	1.941010	5	19			
H	33	-1.897320	-1.855480	1.124860	5	19			
H	34	0.150010	-0.903770	1.277150	23	20			

36midaglizole

N	1	0.059480	-1.992630	-0.733590	9	6	2	0	0	0	0
C	2	0.170180	-2.867280	-1.661330	3	20	3	1	0	0	0
C	3	1.557310	-3.282490	-2.122510	2	21	4	2	0	0	0
C	4	2.591700	-2.686050	-1.512690	2	22	5	3	0	0	0
C	5	2.379570	-1.776090	-0.546340	2	23	6	4	0	0	0
C	6	1.142720	-1.426820	-0.144050	2	7	5	1	0	0	0
C	7	0.931540	-0.380010	0.935260	1	24	9	8	6	0	0
C	8	-0.406400	-0.507820	1.688100	1	26	25	15	7	0	0
C	9	1.146050	1.031300	0.411500	2	14	10	7	0	0	0
C	10	0.804230	1.375940	-0.844220	2	27	11	9	0	0	0
C	11	0.987700	2.630840	-1.285250	2	28	12	10	0	0	0
C	12	1.513620	3.560150	-0.472590	2	29	13	11	0	0	0
C	13	1.851970	3.229360	0.783030	2	30	14	12	0	0	0
C	14	1.666410	1.973580	1.220080	2	31	13	9	0	0	0
C	15	-1.623300	-0.132170	0.874680	3	19	16	8	0	0	0
N	16	-2.519810	-0.916160	0.396340	9	17	15	0	0	0	0
C	17	-3.505050	-0.105110	-0.275110	1	33	32	18	16	0	0
C	18	-3.285900	1.315180	0.288350	1	35	34	19	17	0	0
N	19	-1.907100	1.241490	0.607840	8	36	18	15	0	0	0
H	20	-0.679470	-3.366920	-2.179550	5	2	0	0	0	0	0
H	21	1.690730	-4.032690	-2.919930	5	3	0	0	0	0	0
H	22	3.622980	-2.943960	-1.809390	5	4	0	0	0	0	0
H	23	3.252780	-1.299460	-0.069250	5	5	0	0	0	0	0
H	24	1.731850	-0.580740	1.688460	5	7	0	0	0	0	0
H	25	-0.399850	0.149180	2.589540	5	8	0	0	0	0	0
H	26	-0.533260	-1.552090	2.058920	5	8	0	0	0	0	0
H	27	0.362370	0.631300	-1.526540	5	10	0	0	0	0	0
H	28	0.702590	2.899710	-2.317240	5	11	0	0	0	0	0
H	29	1.663570	4.592320	-0.833950	5	12	0	0	0	0	0
H	30	2.280700	3.991040	1.457260	5	13	0	0	0	0	0
H	31	1.944080	1.718830	2.256980	5	14	0	0	0	0	0
H	32	-4.533640	-0.488850	-0.081160	5	17	0	0	0	0	0
H	33	-3.308500	-0.129030	-1.373600	5	17	0	0	0	0	0
H	34	-3.871980	1.471360	1.225610	5	18	0	0	0	0	0
H	35	-3.492500	2.131120	-0.442700	5	18	0	0	0	0	0
H	36	-1.535480	1.955960	1.218880	23	19	0	0	0	0	0

29mpv1

N	1	-1.479100	-1.694200	2.919650	9	5	2		
C	2	-2.477950	-2.607600	2.786140	2	16	3	1	
N	3	-2.994710	-2.611030	1.446330	8	17	4	2	
C	4	-2.177970	-1.595350	0.852370	2	18	5	3	
C	5	-1.297730	-1.068200	1.714740	2	12	4	1	
C	6	-0.306670	0.530940	0.051600	2	12	11	7	
C	7	-1.077440	1.600730	-0.217960	2	19	8	6	
C	8	-1.143060	2.103850	-1.457770	2	20	9	7	
C	9	-0.434130	1.533160	-2.440570	2	21	10	8	
C	10	0.335600	0.457280	-2.195610	2	13	11	9	
C	11	0.399650	-0.052300	-0.944520	2	10	6	14	
C	12	-0.273770	0.005250	1.475800	1	22	15	6	5
C	13	1.118320	-0.140570	-3.347630	1	25	24	23	10
C	14	1.247710	-1.278870	-0.658210	1	11	26	28	27
H	15	0.737630	-0.385620	1.731170	5	12			
H	16	-2.870630	-3.282830	3.562830	5	2			
H	17	-3.990640	-2.420430	1.392040	23	3			
H	18	-2.318180	-1.338650	-0.209920	5	4			
H	19	-1.670830	2.078390	0.579440	5	7			
H	20	-1.776980	2.982960	-1.668130	5	8			
H	21	-0.493900	1.956860	-3.457440	5	9			
O	22	-0.484230	1.039870	2.409000	6	12	29		
H	23	2.194640	-0.255630	-3.084780	5	13			
H	24	0.696290	-1.130460	-3.635390	5	13			
H	25	1.095150	0.495250	-4.261750	5	13			
H	26	1.456780	-1.901110	-1.555130	5	14			
H	27	0.743570	-1.983160	0.040440	5	14			
H	28	2.225840	-0.973840	-0.221390	5	14			
H	29	-0.548480	0.650290	3.298500	21	22			

28mpv1180

N	1	-2.616610	-1.296420	0.689350	9	5	2		
C	2	-3.341570	-2.424710	0.917170	2	16	3	1	
N	3	-2.663060	-3.288860	1.840980	8	17	4	2	
C	4	-1.481080	-2.520080	2.091060	2	18	5	3	
C	5	-1.462700	-1.356690	1.424820	2	12	4	1	
C	6	0.662190	-0.541570	2.497410	2	12	11	7	
C	7	1.874350	-0.952680	2.079930	2	19	8	6	
C	8	2.860380	-1.192330	2.953960	2	20	9	7	
C	9	2.636520	-1.020780	4.263070	2	21	10	8	
C	10	1.430530	-0.612020	4.694830	2	13	11	9	
C	11	0.428040	-0.368410	3.820270	2	10	6	14	
C	12	-0.397160	-0.297820	1.437050	1	22	15	6	5
C	13	1.259980	-0.439770	6.220120	3	23	10	24	
C	14	-0.931560	0.084450	4.320310	1	11	25	27	26
H	15	-0.851710	0.709000	1.579330	5	12			
H	16	-4.320110	-2.687090	0.484740	5	2			
H	17	-2.478640	-4.216940	1.472470	23	3			
H	18	-0.716370	-2.914440	2.779310	5	4			
H	19	2.072820	-1.101120	1.004890	5	7			
H	20	3.849730	-1.529180	2.597910	5	8			
H	21	3.459090	-1.222280	4.969340	5	9			
H	22	0.042090	-0.267370	0.413500	5	12			
O	23	2.316770	-0.706630	6.988460	6	13	28		
O	24	0.255840	-0.086150	6.791640	7	13			
H	25	-1.370430	-0.678770	5.002260	5	14			
H	26	-1.701110	0.232300	3.534210	5	14			
H	27	-0.850870	1.065270	4.841550	5	14			
H	28	2.089380	-0.523900	7.914820	21	23			

29mpv1181

N	1	-2.502810	-1.400090	0.525280	9	5	2		
C	2	-3.220420	-2.535490	0.739800	2	16	3	1	
N	3	-2.610250	-3.337460	1.762280	8	17	4	2	
C	4	-1.473910	-2.526220	2.082580	2	18	5	3	
C	5	-1.418310	-1.396470	1.362560	2	12	4	1	
C	6	0.671720	-0.540450	2.480490	2	12	11	7	
C	7	1.856200	-1.041300	2.083330	2	19	8	6	
C	8	2.836520	-1.268550	2.967560	2	20	9	7	
C	9	2.633680	-0.991700	4.262310	2	21	10	8	
C	10	1.456320	-0.493320	4.680840	2	13	11	9	
C	11	0.464870	-0.266980	3.789240	2	10	6	14	
C	12	-0.389090	-0.303720	1.421200	1	22	15	6	5
C	13	1.297630	-0.195360	6.158000	1	25	24	23	10
C	14	-0.867810	0.278650	4.269760	1	11	26	28	27
H	15	-0.888080	0.678490	1.585650	5	12			
H	16	-4.149790	-2.842740	0.234590	5	2			
H	17	-2.371420	-4.276180	1.457480	23	3			
H	18	-0.769770	-2.865020	2.859410	5	4			
H	19	2.034010	-1.272920	1.019390	5	7			
H	20	3.804560	-1.679500	2.631610	5	8			
H	21	3.446540	-1.180720	4.983960	5	9			
H	22	0.069520	-0.224530	0.408670	5	12			
O	23	0.601650	-1.237780	6.799530	6	13	29		
H	24	2.275210	-0.092450	6.683240	5	13			
H	25	0.736170	0.747690	6.344520	5	13			
H	26	-1.169070	-0.150750	5.250840	5	14			
H	27	-1.721940	0.033320	3.602510	5	14			
H	28	-0.814260	1.387160	4.363860	5	14			
H	29	1.097300	-2.064400	6.671140	21	23			

31mpv1440- medetomidine r form (mpv785- d isomer)

N	1	-2.500180	-1.818390	0.232690	9	5	2	0	0	0	0
C	2	-2.570260	-3.165060	0.056240	2	16	3	1	0	0	0
N	3	-1.417870	-3.811210	0.617710	8	17	4	2	0	0	0
C	4	-0.701530	-2.673890	1.112850	2	18	5	3	0	0	0
C	5	-1.337430	-1.514600	0.890300	2	12	4	1	0	0	0
C	6	-0.461540	0.655520	0.045540	2	12	11	7	0	0	0
C	7	-1.437280	1.078670	-0.780190	2	19	8	6	0	0	0
C	8	-1.156180	1.785530	-1.882320	2	20	9	7	0	0	0
C	9	0.118330	2.076840	-2.170370	2	21	10	8	0	0	0
C	10	1.113850	1.660740	-1.366850	2	13	11	9	0	0	0
C	11	0.827920	0.944010	-0.254760	2	10	6	14	0	0	0
C	12	-0.870140	-0.137810	1.284370	1	22	15	6	5	0	0
C	13	2.533990	2.026420	-1.752360	1	25	24	23	10	0	0
C	14	1.945110	0.458940	0.652830	1	11	26	28	27	0	0
H	15	-0.002090	-0.276330	1.966490	5	12	0	0	0	0	0
H	16	-3.377630	-3.732900	-0.432670	5	2	0	0	0	0	0
H	17	-0.893870	-4.366360	-0.051900	23	3	0	0	0	0	0
H	18	0.265730	-2.817880	1.620810	5	4	0	0	0	0	0
H	19	-2.492550	0.847520	-0.563450	5	7	0	0	0	0	0
H	20	-1.968740	2.126020	-2.547770	5	8	0	0	0	0	0
H	21	0.339430	2.661180	-3.079620	5	9	0	0	0	0	0
C	22	-1.925340	0.576800	2.146750	1	12	29	30	31	0	0
H	23	3.030850	2.603350	-0.939230	5	13	0	0	0	0	0
H	24	3.127570	1.112820	-1.984460	5	13	0	0	0	0	0
H	25	2.586510	2.670560	-2.659370	5	13	0	0	0	0	0
H	26	1.885870	-0.643870	0.797350	5	14	0	0	0	0	0
H	27	1.895110	0.972430	1.640120	5	14	0	0	0	0	0
H	28	2.972370	0.633600	0.268800	5	14	0	0	0	0	0
H	29	-2.907260	0.687480	1.634190	5	22	0	0	0	0	0
H	30	-2.120620	0.010380	3.087140	5	22	0	0	0	0	0
H	31	-1.576570	1.595220	2.436340	5	22	0	0	0	0	0

31MPV785E- MEDETOMIDINE- MPV1441

N	1	-1.122080	-0.944610	-0.539930	9	5	2	0	0	0	0
C	2	-0.800790	-2.235970	-0.820450	2	11	3	1	0	0	0
N	3	-0.806800	-3.031080	0.374130	8	12	4	2	0	0	0
C	4	-1.158960	-2.036950	1.343340	2	13	5	3	0	0	0
C	5	-1.342790	-0.821030	0.807990	2	10	4	1	0	0	0
H	6	-2.662400	0.760030	0.976680	5	10	0	0	0	0	0
H	7	-2.390910	1.239960	3.449820	5	14	0	0	0	0	0
H	8	-2.887930	-0.452910	3.136840	5	14	0	0	0	0	0
H	9	-1.177800	-0.075170	3.571870	5	14	0	0	0	0	0
C	10	-1.726830	0.462350	1.502380	1	14	15	6	5	0	0
H	11	-0.568830	-2.666780	-1.807330	5	2	0	0	0	0	0
H	12	0.078240	-3.491960	0.562450	23	3	0	0	0	0	0
H	13	-1.252390	-2.328950	2.401260	5	4	0	0	0	0	0
C	14	-2.060400	0.279420	2.991690	1	10	7	8	9	0	0
C	15	-0.644510	1.526620	1.351130	2	20	16	10	0	0	0
C	16	0.633680	1.153630	1.548720	2	23	17	15	0	0	0
C	17	1.633910	2.037740	1.439840	2	24	18	16	0	0	0
C	18	1.357520	3.311820	1.133590	2	25	19	17	0	0	0
C	19	0.087180	3.710860	0.940970	2	21	20	18	0	0	0
C	20	-0.922970	2.817690	1.053040	2	19	15	22	0	0	0
C	21	-0.157090	5.166560	0.595210	1	28	27	26	19	0	0
C	22	-2.363290	3.256740	0.856330	1	20	29	31	30	0	0
H	23	0.875700	0.109190	1.807700	5	16	0	0	0	0	0
H	24	2.678280	1.718670	1.602310	5	17	0	0	0	0	0
H	25	2.188990	4.031510	1.045380	5	18	0	0	0	0	0
H	26	-0.742970	5.260250	-0.347570	5	21	0	0	0	0	0
H	27	-0.693120	5.682900	1.424010	5	21	0	0	0	0	0
H	28	0.784890	5.736000	0.425570	5	21	0	0	0	0	0
H	29	-2.516430	4.357010	0.859410	5	22	0	0	0	0	0
H	30	-3.016020	2.891740	1.680850	5	22	0	0	0	0	0
H	31	-2.750900	2.879120	-0.117310	5	22	0	0	0	0	0

31mpv2

N	1	-2.728130	-1.543270	2.409670	9	5	2	0	0	0	0
C	2	-3.027900	-2.855100	2.212980	2	16	3	1	0	0	0
N	3	-2.182800	-3.423300	1.200930	8	17	4	2	0	0	0
C	4	-1.383540	-2.283430	0.863320	2	18	5	3	0	0	0
C	5	-1.714400	-1.186430	1.559870	2	12	4	1	0	0	0
C	6	-0.499660	0.492850	0.104150	2	12	11	7	0	0	0
C	7	0.827890	0.722120	-0.048190	2	19	8	6	0	0	0
C	8	1.330710	1.017770	-1.261130	2	20	9	7	0	0	0
C	9	0.533980	1.092370	-2.333840	2	21	10	8	0	0	0
C	10	-0.777430	0.868680	-2.187830	2	13	11	9	0	0	0
C	11	-1.303310	0.571080	-0.984530	2	10	6	14	0	0	0
C	12	-1.062160	0.168480	1.488530	1	22	15	6	5	0	0
H	13	-1.429310	0.935260	-3.075850	5	10	0	0	0	0	0
C	14	-2.803410	0.341960	-0.968420	1	11	23	25	24	0	0
H	15	-0.255310	0.066100	2.246950	5	12	0	0	0	0	0
H	16	-3.792630	-3.450550	2.736350	5	2	0	0	0	0	0
H	17	-2.693180	-3.812960	0.414260	23	3	0	0	0	0	0
H	18	-0.590910	-2.379480	0.103870	5	4	0	0	0	0	0
C	19	1.806020	0.666470	1.110910	1	7	29	30	31	0	0
H	20	2.410270	1.205270	-1.389410	5	8	0	0	0	0	0
H	21	0.952650	1.336660	-3.325790	5	9	0	0	0	0	0
C	22	-1.941980	1.311450	2.024360	1	12	26	27	28	0	0
H	23	-3.334000	1.321250	-0.982120	5	14	0	0	0	0	0
H	24	-3.183570	-0.241090	-0.105050	5	14	0	0	0	0	0
H	25	-3.130840	-0.233640	-1.864400	5	14	0	0	0	0	0
H	26	-2.876570	1.457770	1.440570	5	22	0	0	0	0	0
H	27	-2.247430	1.129610	3.081030	5	22	0	0	0	0	0
H	28	-1.385160	2.277000	2.006010	5	22	0	0	0	0	0
H	29	1.848950	-0.358910	1.544380	5	19	0	0	0	0	0
H	30	2.850130	0.915760	0.814420	5	19	0	0	0	0	0
H	31	1.532910	1.404590	1.899380	5	19	0	0	0	0	0

28mpv207

N	1	-2.444090	-1.434870	0.474740	9	5	2		
C	2	-3.107510	-2.612020	0.630850	2	16	3	1	
N	3	-2.481440	-3.419540	1.639270	8	17	4	2	
C	4	-1.398080	-2.562900	2.019040	2	18	5	3	
C	5	-1.381650	-1.407480	1.339040	2	12	4	1	
C	6	0.659310	-0.522970	2.511640	2	12	11	7	
C	7	1.828710	-1.106940	2.164180	2	19	8	6	
C	8	2.768560	-1.328700	3.101130	2	20	9	7	
C	9	2.557970	-0.979090	4.377220	2	21	10	8	
C	10	1.396940	-0.406700	4.722590	2	13	11	9	
C	11	0.444290	-0.175640	3.801030	2	10	6	14	
C	12	-0.411270	-0.267820	1.464060	1	22	15	6	5
H	13	1.232060	-0.126990	5.776950	5	10			
C	14	-0.854150	0.461900	4.254640	1	11	26	28	27
H	15	-0.980800	0.661610	1.687900	5	12			
H	16	-4.007470	-2.947070	0.091240	5	2			
H	17	-2.185340	-4.332050	1.306390	23	3			
H	18	-0.697480	-2.893100	2.802690	5	4			
C	19	2.117730	-1.538460	0.740120	1	7	23	24	25
H	20	3.726160	-1.803880	2.828590	5	8			
H	21	3.334290	-1.165300	5.139810	5	9			
H	22	0.033920	-0.070000	0.463820	5	12			
H	23	2.289100	-0.650220	0.090330	5	19			
H	24	3.026370	-2.177360	0.659610	5	19			
H	25	1.282090	-2.145700	0.323750	5	19			
H	26	-0.957100	0.486420	5.363290	5	14			
H	27	-1.738080	-0.103370	3.881670	5	14			
H	28	-0.914700	1.516040	3.900160	5	14			

28mpv253---detomidine

N	1	-2.435160	-1.456250	0.448050	9	5	2		
C	2	-3.114990	-2.619310	0.636970	2	16	3	1	
N	3	-2.482810	-3.421690	1.645580	8	17	4	2	
C	4	-1.377240	-2.578420	1.988580	2	18	5	3	
C	5	-1.355620	-1.433640	1.290820	2	12	4	1	
C	6	0.674090	-0.543100	2.464270	2	12	11	7	
C	7	1.837440	-1.122210	2.115290	2	19	8	6	
C	8	2.788000	-1.352740	3.030540	2	20	9	7	
C	9	2.575510	-1.000620	4.305590	2	21	10	8	
C	10	1.417470	-0.423970	4.675810	2	13	11	9	
C	11	0.456300	-0.194120	3.752730	2	10	6	14	
C	12	-0.357970	-0.314080	1.375820	1	22	15	6	5
C	13	1.239660	-0.040600	6.131230	1	25	24	23	10
C	14	-0.863180	0.439580	4.154710	1	11	26	28	27
H	15	-0.890620	0.651660	1.529460	5	12			
H	16	-4.031170	-2.947330	0.120830	5	2			
H	17	-2.209890	-4.344670	1.321880	23	3			
H	18	-0.665450	-2.910220	2.761430	5	4			
H	19	2.019970	-1.416820	1.067800	5	7			
H	20	3.739860	-1.828160	2.735950	5	8			
H	21	3.365930	-1.192700	5.050860	5	9			
H	22	0.131510	-0.218000	0.379250	5	12			
H	23	0.926390	1.023790	6.229970	5	13			
H	24	0.485030	-0.698440	6.619620	5	13			
H	25	2.179120	-0.137580	6.721490	5	13			
H	26	-1.110180	0.317880	5.231600	5	14			
H	27	-1.728250	-0.021460	3.628260	5	14			
H	28	-0.845790	1.530490	3.930770	5	14			

31mpv295

N	1	-3.106410	-1.098680	1.037470	9	5	2			
C	2	-3.922580	-1.677410	0.114800	2	16	3	1		
N	3	-3.401300	-2.948220	-0.303980	8	17	4	2		
C	4	-2.206280	-3.006500	0.483190	2	18	5	3		
C	5	-2.041790	-1.929080	1.263220	2	4	1	29		
C	6	1.082620	-0.192450	2.723300	2	12	11	7		
C	7	2.278300	-0.736180	2.396920	2	19	8	6		
C	8	3.339460	-0.550670	3.203330	2	20	9	7		
C	9	3.228090	0.169890	4.326970	2	21	10	8		
C	10	2.046170	0.712680	4.647710	2	13	11	9		
C	11	0.971770	0.539690	3.855880	2	10	6	14		
C	12	-0.125010	-0.402310	1.819490	1	22	15	6	29	
H	13	1.966860	1.307530	5.573440	5	10				
C	14	-0.334670	1.184130	4.277390	1	11	23	25	24	
H	15	-0.798580	0.484470	1.837500	5	12				
H	16	-4.866300	-1.274410	-0.285670	5	2				
H	17	-3.237370	-3.012970	-1.304040	23	3				
H	18	-1.541910	-3.882160	0.404540	5	4				
C	19	2.478300	-1.560420	1.139270	1	7	26	27	28	
H	20	4.318650	-0.989510	2.946960	5	8				
H	21	4.104340	0.317860	4.982130	5	9				
H	22	0.187300	-0.470180	0.752620	5	12				
H	23	-0.296810	1.601600	5.309160	5	14				
H	24	-1.175290	0.455550	4.278810	5	14				
H	25	-0.585710	2.031260	3.599280	5	14				
H	26	2.442120	-0.906700	0.238230	5	19				
H	27	3.462700	-2.080720	1.116610	5	19				
H	28	1.713950	-2.362590	1.039590	5	19				
C	29	-0.907970	-1.666620	2.210780	1	5	12	30	31	
H	30	-1.330200	-1.570910	3.237030	5	29				
H	31	-0.231750	-2.551870	2.226610	5	29				

31NPV295A

N	1	-2.224660	-1.642440	-0.021230	9	5	2	0	0	0	0
C	2	-3.505640	-1.989790	-0.321630	2	16	3	1	0	0	0
N	3	-4.130670	-2.649180	0.790620	8	17	4	2	0	0	0
C	4	-3.055580	-2.630130	1.737090	2	18	5	3	0	0	0
C	5	-1.949660	-2.043400	1.258580	2	4	1	29	0	0	0
C	6	0.993530	-0.131310	2.872880	2	12	11	7	0	0	0
C	7	0.980690	0.016110	4.218110	2	19	8	6	0	0	0
C	8	2.135730	0.211740	4.880280	2	20	9	7	0	0	0
C	9	3.301570	0.264980	4.222910	2	21	10	8	0	0	0
C	10	3.314390	0.123370	2.890980	2	13	11	9	0	0	0
C	11	2.171160	-0.072970	2.208740	2	10	6	14	0	0	0
C	12	-0.307170	-0.352310	2.112730	1	22	15	6	29	0	0
H	13	4.279820	0.172880	2.359380	5	10	0	0	0	0	0
C	14	2.258630	-0.221020	0.701900	1	11	23	25	24	0	0
H	15	-1.151180	0.177720	2.609870	5	12	0	0	0	0	0
H	16	-4.040550	-1.809500	-1.267540	5	2	0	0	0	0	0
H	17	-4.470560	-3.581340	0.574470	23	3	0	0	0	0	0
H	18	-3.199890	-3.067970	2.737980	5	4	0	0	0	0	0
C	19	-0.302300	-0.029940	5.025780	1	7	26	27	28	0	0
H	20	2.136520	0.333480	5.976780	5	8	0	0	0	0	0
H	21	4.244280	0.427020	4.774260	5	9	0	0	0	0	0
H	22	-0.261900	0.121680	1.105950	5	12	0	0	0	0	0
H	23	3.306330	-0.324370	0.338690	5	14	0	0	0	0	0
H	24	1.833710	0.677080	0.198580	5	14	0	0	0	0	0
H	25	1.725500	-1.128490	0.341760	5	14	0	0	0	0	0
H	26	-0.912270	-0.929150	4.786840	5	19	0	0	0	0	0
H	27	-0.119650	-0.074460	6.123470	5	19	0	0	0	0	0
H	28	-0.910200	0.884660	4.840120	5	19	0	0	0	0	0
C	29	-0.645890	-1.845890	1.975840	1	5	12	30	31	0	0
H	30	-0.699170	-2.325890	2.979830	5	29	0	0	0	0	0
H	31	0.146090	-2.383170	1.406100	5	29	0	0	0	0	0

25mpv3

N	1	-2.453380	-1.806680	0.196090	9	5	2		
C	2	-2.508850	-3.155260	0.025080	2	16	3	1	
N	3	-1.372010	-3.792740	0.627970	8	17	4	2	
C	4	-0.679590	-2.649640	1.143920	2	18	5	3	
C	5	-1.315230	-1.496830	0.892080	2	12	4	1	
C	6	-0.510220	0.688340	0.058760	2	12	11	7	
C	7	-1.465760	1.316850	-0.648520	2	19	8	6	
C	8	-1.143830	2.030990	-1.738300	2	20	9	7	
C	9	0.136940	2.122100	-2.129380	2	21	10	8	
C	10	1.103120	1.497190	-1.433570	2	13	11	9	
C	11	0.769830	0.782740	-0.343660	2	10	6	14	
C	12	-0.877830	-0.116290	1.286450	1	22	15	6	5
C	13	2.551080	1.584840	-1.857520	1	25	24	23	10
H	14	1.560870	0.267590	0.226400	5	11			
H	15	-0.013130	-0.175850	1.987280	5	12			
H	16	-3.295400	-3.730410	-0.488640	5	2			
H	17	-0.822160	-4.346600	-0.021700	23	3			
H	18	0.270920	-2.783760	1.685050	5	4			
H	19	-2.521460	1.247590	-0.335370	5	7			
H	20	-1.933730	2.544520	-2.313660	5	8			
H	21	0.390230	2.712260	-3.026330	5	9			
H	22	-1.701990	0.377990	1.850900	5	12			
H	23	3.160240	2.058310	-1.053950	5	13			
H	24	2.958490	0.567170	-2.056040	5	13			
H	25	2.693170	2.186950	-2.783670	5	13			

29mpv305t- mpv6t

N	1	-3.686130	-1.683690	2.336440	9	5	2		
C	2	-3.681350	-2.629130	3.311720	2	15	3	1	
N	3	-2.334830	-2.979480	3.659620	8	16	4	2	
C	4	-1.605290	-2.129510	2.765080	2	17	5	3	
C	5	-2.396500	-1.369060	1.992430	2	4	1	21	
C	6	-0.419260	0.783540	-0.241160	2	12	11	7	
C	7	0.935150	0.883730	-0.372850	2	18	8	6	
C	8	1.489010	1.741160	-1.251110	2	19	9	7	
C	9	0.728920	2.522360	-2.022570	2	20	10	8	
C	10	-0.598920	2.435290	-1.905000	2	13	11	9	
C	11	-1.181070	1.585670	-1.034300	2	10	6	14	
C	12	-0.873980	-0.111050	0.675790	2	21	6	28	
H	13	-1.211420	3.088120	-2.549870	5	10			
C	14	-2.698460	1.640590	-1.052710	1	11	22	24	23
H	15	-4.552810	-3.088470	3.804570	5	2			
H	16	-2.127480	-3.967250	3.547860	23	3			
H	17	-0.504430	-2.166100	2.791170	5	4			
C	18	1.936170	0.062020	0.433610	1	7	25	26	27
H	19	2.584970	1.816910	-1.352200	5	8			
H	20	1.187960	3.224020	-2.741100	5	9			
C	21	-2.122620	-0.454030	1.047740	2	12	5	29	
H	22	-3.099970	1.985080	-0.072740	5	14			
H	23	-3.131430	0.670010	-1.385510	5	14			
H	24	-3.112180	2.376260	-1.779160	5	14			
H	25	1.817960	-1.028730	0.237790	5	18			
H	26	2.998070	0.282920	0.181040	5	18			
H	27	1.852090	0.275650	1.524180	5	18			
H	28	-0.114060	-0.670210	1.231130	5	12			
H	29	-3.002450	0.004300	0.592480	5	21			

31mpv327

N	1	-3.174250	-1.137580	1.106180	9	5	2		
C	2	-4.027570	-1.735480	0.230800	2	16	3	1	
N	3	-3.535850	-3.026690	-0.160340	8	17	4	2	
C	4	-2.316000	-3.074280	0.589070	2	18	5	3	
C	5	-2.111970	-1.973090	1.325670	2	4	1	29	
C	6	1.004580	-0.185080	2.702800	2	12	11	7	
C	7	2.198460	-0.733260	2.418230	2	19	8	6	
C	8	3.269520	-0.531800	3.208150	2	20	9	7	
C	9	3.144410	0.235060	4.311440	2	21	10	8	
C	10	1.949320	0.783510	4.597250	2	13	11	9	
C	11	0.887860	0.576650	3.802980	2	10	6	14	
C	12	-0.188120	-0.427450	1.799440	1	22	15	6	29
H	13	1.830090	1.412360	5.495830	5	10			
H	14	-0.083080	1.033980	4.058910	5	11			
H	15	-0.868760	0.456230	1.820770	5	12			
H	16	-4.979170	-1.333820	-0.151990	5	2			
H	17	-3.406030	-3.128070	-1.162360	23	3			
H	18	-1.666380	-3.961710	0.519990	5	4			
H	19	2.296720	-1.361820	1.517790	5	7			
C	20	4.590990	-1.176300	2.845990	1	8	23	24	25
C	21	4.321040	0.494520	5.228090	1	9	26	27	28
H	22	0.150590	-0.531370	0.741450	5	12			
H	23	5.311940	-0.404820	2.491720	5	20			
H	24	5.032600	-1.710940	3.717210	5	20			
H	25	4.492340	-1.931890	2.033730	5	20			
H	26	4.584450	-0.430270	5.790070	5	21			
H	27	5.212330	0.835010	4.653930	5	21			
H	28	4.111730	1.288130	5.980920	5	21			
C	29	-0.947120	-1.691320	2.229790	1	5	12	30	31
H	30	-1.333090	-1.571200	3.269090	5	29			
H	31	-0.255010	-2.566010	2.228050	5	29			

31MPV327A

N	1	-3.244820	-1.361990	1.434460	9	5	2	0	0	0	0
C	2	-4.135800	-1.846780	0.527070	2	16	3	1	0	0	0
N	3	-3.548740	-2.901230	-0.250980	8	17	4	2	0	0	0
C	4	-2.235520	-2.940850	0.319790	2	18	5	3	0	0	0
C	5	-2.064740	-2.043900	1.301230	2	4	1	29	0	0	0
C	6	0.948580	-0.171230	2.804730	2	12	11	7	0	0	0
C	7	0.899850	0.001110	4.137210	2	19	8	6	0	0	0
C	8	2.018920	0.178950	4.864250	2	20	9	7	0	0	0
C	9	3.217910	0.184510	4.244520	2	21	10	8	0	0	0
C	10	3.267530	0.012070	2.910880	2	13	11	9	0	0	0
C	11	2.146110	-0.164940	2.195730	2	10	6	14	0	0	0
C	12	-0.326480	-0.370440	2.008570	1	22	15	6	29	0	0
H	13	4.239430	0.013310	2.388850	5	10	0	0	0	0	0
H	14	2.213750	-0.307150	1.103730	5	11	0	0	0	0	0
H	15	-1.107230	0.335390	2.378740	5	12	0	0	0	0	0
H	16	-5.176350	-1.519330	0.374010	5	2	0	0	0	0	0
H	17	-3.556460	-2.724220	-1.250860	23	3	0	0	0	0	0
H	18	-1.497350	-3.666790	-0.057550	5	4	0	0	0	0	0
H	19	-0.081590	-0.005130	4.639480	5	7	0	0	0	0	0
C	20	1.911220	0.366130	6.363550	1	8	23	24	25	0	0
C	21	4.503710	0.382940	5.019740	1	9	26	27	28	0	0
H	22	-0.159250	-0.113360	0.935960	5	12	0	0	0	0	0
H	23	2.524360	-0.390400	6.903660	5	20	0	0	0	0	0
H	24	2.254640	1.384590	6.655150	5	20	0	0	0	0	0
H	25	0.868570	0.255680	6.739030	5	20	0	0	0	0	0
H	26	4.473410	1.329960	5.604740	5	21	0	0	0	0	0
H	27	4.673700	-0.467890	5.717890	5	21	0	0	0	0	0
H	28	5.399310	0.445640	4.360740	5	21	0	0	0	0	0
C	29	-0.824570	-1.819570	2.117660	1	5	12	30	31	0	0
H	30	-1.060380	-2.067570	3.178880	5	29	0	0	0	0	0
H	31	-0.023180	-2.517930	1.779780	5	29	0	0	0	0	0

26mpv4

N	1	-2.557120	-1.758380	0.436840	9	5	2		
C	2	-2.682350	-3.100270	0.251270	2	16	3	1	
N	3	-1.487780	-3.788530	0.654540	8	17	4	2	
C	4	-0.682630	-2.681260	1.075680	2	18	5	3	
C	5	-1.312950	-1.505630	0.950170	2	12	4	1	
C	6	-0.462820	0.647010	0.040620	2	12	11	7	
C	7	-1.441830	1.222210	-0.680420	2	19	8	6	
C	8	-1.150360	1.918470	-1.790320	2	20	9	7	
C	9	0.123890	2.044400	-2.192100	2	21	10	8	
C	10	1.113950	1.471380	-1.485870	2	13	11	9	
C	11	0.810400	0.775990	-0.375320	2	10	6	14	
C	12	-0.782660	-0.143430	1.292460	1	22	15	6	5
C	13	2.555980	1.596670	-1.920470	1	25	24	23	10
H	14	1.624040	0.304540	0.200640	5	11			
H	15	0.126380	-0.248070	1.928750	5	12			
H	16	-3.558900	-3.638520	-0.142820	5	2			
H	17	-1.067280	-4.343950	-0.084280	23	3			
H	18	0.336570	-2.856360	1.456220	5	4			
H	19	-2.494370	1.125520	-0.366080	5	7			
H	20	-1.960860	2.387860	-2.374720	5	8			
H	21	0.351710	2.618620	-3.106060	5	9			
O	22	-1.709430	0.533990	2.107300	6	12	26		
H	23	3.160040	2.083710	-1.121140	5	13			
H	24	2.986560	0.589650	-2.124210	5	13			
H	25	2.675730	2.204670	-2.845940	5	13			
H	26	-2.603000	0.408310	1.744890	21	22			

28mpv5

N	1	-2.644240	-1.754690	0.673670	9	5	2		
C	2	-2.744060	-3.104960	0.542340	2	16	3	1	
N	3	-1.503860	-3.743380	0.882450	8	17	4	2	
C	4	-0.707570	-2.598110	1.207600	2	18	5	3	
C	5	-1.377930	-1.442880	1.092290	2	12	4	1	
C	6	-0.478820	0.589220	0.015850	2	12	11	7	
C	7	0.809300	0.780510	-0.323870	2	19	8	6	
C	8	1.129650	1.351600	-1.495490	2	20	9	7	
C	9	0.164090	1.737430	-2.343620	2	21	10	8	
C	10	-1.127850	1.550300	-2.023160	2	13	11	9	
C	11	-1.436510	0.976620	-0.846440	2	10	6	14	
C	12	-0.837550	-0.060330	1.342030	1	22	15	6	5
C	13	-2.234200	1.972930	-2.961900	1	25	24	23	10
H	14	-2.497480	0.822050	-0.592930	5	11			
H	15	0.092450	-0.177200	1.948580	5	12			
H	16	-3.628940	-3.680440	0.227460	5	2			
H	17	-1.118590	-4.311640	0.134220	23	3			
H	18	0.342310	-2.732670	1.514230	5	4			
H	19	1.617310	0.468670	0.359400	5	7			
H	20	2.189980	1.504130	-1.762380	5	8			
H	21	0.438150	2.205680	-3.304130	5	9			
C	22	-1.803400	0.782800	2.188520	1	12	26	27	28
H	23	-2.821780	1.084660	-3.288590	5	13			
H	24	-2.923920	2.684920	-2.453530	5	13			
H	25	-1.851970	2.477770	-3.878150	5	13			
H	26	-1.385130	1.799410	2.372870	5	22			
H	27	-2.798870	0.909130	1.705920	5	22			
H	28	-1.980330	0.307190	3.181150	5	22			

28MPV5A

N	1	-2.639020	-1.748760	0.666710	9	5	2	0	0	0	0
C	2	-2.744600	-3.099090	0.540470	2	16	3	1	0	0	0
N	3	-1.510780	-3.741980	0.895040	8	17	4	2	0	0	0
C	4	-0.711730	-2.599150	1.222140	2	18	5	3	0	0	0
C	5	-1.374940	-1.441010	1.095210	2	12	4	1	0	0	0
C	6	-0.482010	0.594090	0.018090	2	12	11	7	0	0	0
C	7	-1.446670	0.990740	-0.831670	2	19	8	6	0	0	0
C	8	-1.131710	1.564140	-2.003590	2	20	9	7	0	0	0
C	9	0.154100	1.745550	-2.341560	2	21	10	8	0	0	0
C	10	1.131760	1.352080	-1.507230	2	13	11	9	0	0	0
C	11	0.803740	0.779090	-0.335460	2	10	6	14	0	0	0
C	12	-0.830670	-0.059790	1.344990	1	22	15	6	5	0	0
C	13	2.587320	1.541670	-1.867220	1	25	24	23	10	0	0
H	14	1.610730	0.456710	0.343190	5	11	0	0	0	0	0
H	15	0.103760	-0.179100	1.944190	5	12	0	0	0	0	0
H	16	-3.629520	-3.671610	0.220340	5	2	0	0	0	0	0
H	17	-1.121480	-4.315790	0.153170	23	3	0	0	0	0	0
H	18	0.334410	-2.737700	1.539580	5	4	0	0	0	0	0
H	19	-2.508820	0.845610	-0.575060	5	7	0	0	0	0	0
H	20	-1.932440	1.885640	-2.692240	5	8	0	0	0	0	0
H	21	0.401690	2.217060	-3.307650	5	9	0	0	0	0	0
C	22	-1.789430	0.780420	2.202380	1	12	26	27	28	0	0
H	23	3.080240	2.219490	-1.133360	5	13	0	0	0	0	0
H	24	3.120120	0.563360	-1.857410	5	13	0	0	0	0	0
H	25	2.726420	1.985430	-2.879260	5	13	0	0	0	0	0
H	26	-1.369680	1.796420	2.386770	5	22	0	0	0	0	0
H	27	-2.788990	0.908010	1.728680	5	22	0	0	0	0	0
H	28	-1.958010	0.301430	3.194830	5	22	0	0	0	0	0

32mpv7

N	1	-3.519990	-1.634760	2.659130	9	5	2		
C	2	-3.454910	-2.778820	3.384460	2	15	3	1	
N	3	-2.168330	-3.387070	3.223190	8	16	4	2	
C	4	-1.550890	-2.451650	2.329120	2	17	5	3	
C	5	-2.337230	-1.413260	1.996970	2	4	1	21	
C	6	-0.438420	0.754480	-0.284900	2	12	11	7	
C	7	0.920290	0.888000	-0.315140	2	18	8	6	
C	8	1.521030	1.762970	-1.144650	2	19	9	7	
C	9	0.809830	2.517500	-1.986310	2	20	10	8	
C	10	-0.516360	2.361550	-2.008000	2	13	11	9	
C	11	-1.139240	1.494240	-1.185140	2	10	6	14	
C	12	-0.934080	-0.131980	0.618940	2	21	6	28	
H	13	-1.094590	2.948720	-2.742420	5	10			
C	14	-2.610930	1.336210	-1.514700	1	11	22	24	23
H	15	-4.238990	-3.217970	4.021360	5	2			
H	16	-2.206880	-4.335510	2.862370	23	3			
H	17	-0.519510	-2.664800	2.005950	5	4			
C	18	1.874380	0.132140	0.606160	1	7	25	26	27
H	19	2.618130	1.879040	-1.143500	5	8			
H	20	1.307980	3.228980	-2.668090	5	9			
C	21	-2.140580	-0.342880	1.197840	2	12	5	29	
H	22	-3.248900	2.129110	-1.064690	5	14			
H	23	-2.971340	0.304490	-1.315260	5	14			
H	24	-2.784130	1.419820	-2.612330	5	14			
H	25	1.907390	-0.951880	0.349390	5	18			
H	26	2.929380	0.481820	0.535940	5	18			
H	27	1.608440	0.271370	1.679510	5	18			
H	28	-0.186040	-0.824140	1.014340	5	12			
C	29	-3.293740	0.639560	1.169650	1	21	30	31	32
H	30	-4.124030	0.329770	0.495990	5	29			
H	31	-3.752760	0.745200	2.178860	5	29			
H	32	-2.942680	1.677370	0.984660	5	29			

31mpv743

N	1	-3.103510	-1.115290	1.067090	9	5	2	0	0	0	0
C	2	-3.951220	-1.693080	0.172940	2	16	3	1	0	0	0
N	3	-3.453730	-2.972080	-0.249720	8	17	4	2	0	0	0
C	4	-2.236200	-3.034930	0.502010	2	18	5	3	0	0	0
C	5	-2.038710	-1.952620	1.267390	2	4	1	29	0	0	0
C	6	1.032800	-0.158450	2.748170	2	12	11	7	0	0	0
C	7	2.217030	-0.725860	2.451000	2	19	8	6	0	0	0
C	8	3.294970	-0.557700	3.235370	2	20	9	7	0	0	0
C	9	3.178940	0.195290	4.341150	2	21	10	8	0	0	0
C	10	2.003490	0.765020	4.647200	2	13	11	9	0	0	0
C	11	0.923720	0.598210	3.860990	2	10	6	14	0	0	0
C	12	-0.138300	-0.399870	1.811310	1	22	15	6	29	0	0
H	13	1.932020	1.379620	5.560620	5	10	0	0	0	0	0
C	14	-0.380510	1.260020	4.254340	1	11	23	25	24	0	0
H	15	-0.838180	0.466740	1.811970	5	12	0	0	0	0	0
H	16	-4.903150	-1.285150	-0.202320	5	2	0	0	0	0	0
H	17	-3.320570	-3.047330	-1.253600	23	3	0	0	0	0	0
H	18	-1.583780	-3.918510	0.413000	5	4	0	0	0	0	0
H	19	2.310420	-1.347120	1.544560	5	7	0	0	0	0	0
C	20	4.605670	-1.212470	2.866090	1	8	26	27	28	0	0
H	21	4.047970	0.349290	5.003120	5	9	0	0	0	0	0
H	22	0.227200	-0.473640	0.759690	5	12	0	0	0	0	0
H	23	-0.350400	1.692680	5.280100	5	14	0	0	0	0	0
H	24	-1.223910	0.533640	4.251510	5	14	0	0	0	0	0
H	25	-0.616660	2.095240	3.556380	5	14	0	0	0	0	0
H	26	4.959200	-0.837780	1.878370	5	20	0	0	0	0	0
H	27	5.411330	-1.011210	3.608310	5	20	0	0	0	0	0
H	28	4.481350	-2.317580	2.800540	5	20	0	0	0	0	0
C	29	-0.879780	-1.692560	2.184940	1	5	12	30	31	0	0
H	30	-1.273430	-1.628890	3.225590	5	29	0	0	0	0	0
H	31	-0.175030	-2.556300	2.150010	5	29	0	0	0	0	0

31mpv750

N	1	-2.321500	-1.608780	2.730180	9	5	2		
C	2	-2.451520	-2.958790	2.626260	2	16	3	1	
N	3	-1.761180	-3.450000	1.463370	8	17	4	2	
C	4	-1.243440	-2.219600	0.935300	2	18	5	3	
C	5	-1.577100	-1.152480	1.675180	2	12	4	1	
C	6	-0.569820	0.515160	0.087000	2	12	11	7	
C	7	0.776770	0.536410	-0.036440	2	19	8	6	
C	8	1.333150	0.738940	-1.244710	2	20	9	7	
C	9	0.567230	0.917700	-2.329310	2	21	10	8	
C	10	-0.766680	0.889960	-2.208100	2	13	11	9	
C	11	-1.343060	0.689640	-1.009080	2	10	6	14	
C	12	-1.216660	0.286900	1.442930	1	15	6	5	28
H	13	-1.387960	1.033850	-3.108320	5	10			
C	14	-2.857170	0.655840	-0.937000	1	11	22	24	23
H	15	-0.575590	0.632070	2.283860	5	12			
H	16	-2.980190	-3.629470	3.322480	5	2			
C	17	-2.504080	-4.278430	0.572010	1	3	29	30	31
H	18	-0.634610	-2.233500	0.016700	5	4			
C	19	1.694170	0.324160	1.151200	1	7	25	26	27
H	20	2.430480	0.758560	-1.356840	5	8			
H	21	1.032200	1.082520	-3.317000	5	9			
H	22	-3.244180	1.573780	-0.438960	5	14			
H	23	-3.220120	-0.241770	-0.387170	5	14			
H	24	-3.334770	0.608040	-1.941930	5	14			
H	25	1.414100	-0.593090	1.717620	5	19			
H	26	2.758570	0.185030	0.854580	5	19			
H	27	1.662190	1.205070	1.832050	5	19			
H	28	-2.137680	0.904000	1.541050	5	12			
H	29	-2.846700	-5.194050	1.106000	5	17			
H	30	-3.390700	-3.734670	0.170180	5	17			
H	31	-1.855080	-4.596080	-0.275830	5	17			

29mpv830

N	1	-2.515970	-1.388700	0.589660	9	5	2		
C	2	-3.214500	-2.540350	0.778020	2	16	3	1	
N	3	-2.536640	-3.407230	1.700880	8	17	4	2	
C	4	-1.382090	-2.613570	1.998670	2	18	5	3	
C	5	-1.380800	-1.438110	1.354840	2	12	4	1	
C	6	0.695330	-0.568770	2.482680	2	12	11	7	
C	7	1.899910	-1.098650	2.165250	2	19	8	6	
C	8	2.821450	-1.295340	3.125800	2	20	9	7	
C	9	2.560660	-0.975930	4.399900	2	21	10	8	
C	10	1.365340	-0.462250	4.717510	2	13	11	9	
C	11	0.428850	-0.257360	3.772830	2	10	6	14	
C	12	-0.347740	-0.347690	1.397620	1	22	15	6	5
H	13	1.157840	-0.209250	5.771190	5	10			
C	14	-0.904340	0.307250	4.224660	1	11	26	28	27
O	15	-0.976600	0.904410	1.538100	6	12	29		
H	16	-4.174520	-2.819590	0.315720	5	2			
H	17	-2.317810	-4.321480	1.316930	23	3			
H	18	-0.621800	-3.000410	2.696050	5	4			
C	19	2.258450	-1.501020	0.747670	1	7	23	24	25
H	20	3.806170	-1.725190	2.875480	5	8			
H	21	3.321790	-1.140800	5.182470	5	9			
H	22	0.105890	-0.283710	0.384170	5	12			
H	23	2.381350	-0.601150	0.102780	5	19			
H	24	3.215320	-2.067640	0.687250	5	19			
H	25	1.483690	-2.172700	0.312350	5	19			
H	26	-1.082390	0.152560	5.313200	5	14			
H	27	-1.765580	-0.183000	3.718730	5	14			
H	28	-0.942860	1.405110	4.041750	5	14			
H	29	-1.737950	0.944900	0.933670	21	15			

32napactadine

C	1	-2.767410	-0.279100	-2.229180	2	6	2	17	
C	2	-2.735210	-1.249910	-3.155750	2	3	1	18	
C	3	-1.569120	-1.830310	-3.477510	2	4	2	19	
C	4	-0.435510	-1.439380	-2.873710	2	5	3	20	
C	5	-0.461710	-0.466400	-1.943510	2	7	6	4	
C	6	-1.633210	0.114530	-1.620300	2	10	5	1	
C	7	0.671850	-0.070310	-1.334930	2	8	5	21	
C	8	0.652190	0.897700	-0.401400	2	11	9	7	
C	9	-0.521650	1.471740	-0.085540	2	10	8	22	
C	10	-1.656340	1.085270	-0.689170	2	9	6	23	
C	11	1.924730	1.345590	0.286450	1	12	8	24	25
C	12	2.054460	0.748750	1.666310	2	15	13	11	
N	13	1.250480	1.213430	2.652380	9	14	12		
C	14	1.057340	0.630440	3.928490	1	13	26	27	28
N	15	2.772020	-0.478760	1.874180	8	16	12	29	
C	16	2.144590	-1.709110	1.535310	1	15	30	31	32
H	17	-3.735750	0.187340	-1.976060	5	1			
H	18	-3.667190	-1.571160	-3.652670	5	2			
H	19	-1.542380	-2.628910	-4.239250	5	3			
H	20	0.514360	-1.928700	-3.152430	5	4			
H	21	1.634380	-0.540410	-1.598830	5	7			
H	22	-0.557730	2.269190	0.676090	5	9			
H	23	-2.605230	1.575470	-0.408640	5	10			
H	24	1.934780	2.457130	0.370180	5	11			
H	25	2.824400	1.078740	-0.314580	5	11			
H	26	0.407560	1.295230	4.540320	5	14			
H	27	2.029430	0.507260	4.458000	5	14			
H	28	0.552900	-0.357910	3.840800	5	14			
H	29	3.719130	-0.460100	1.506960	23	15			
H	30	2.752660	-2.551940	1.935130	5	16			
H	31	2.070730	-1.817300	0.430110	5	16			
H	32	1.125320	-1.767610	1.979110	5	16			

32napamezole

C	1	-2.758200	-0.259510	-2.398570	2	6	2	17	
C	2	-2.692020	-1.235150	-3.316820	2	3	1	18	
C	3	-1.520810	-1.843810	-3.553540	2	4	2	19	
C	4	-0.422160	-1.468130	-2.879800	2	5	3	20	
C	5	-0.476040	-0.474440	-1.970720	2	7	6	4	
C	6	-1.658620	0.123730	-1.724360	2	10	5	1	
C	7	0.647260	-0.115270	-1.319560	2	8	5	21	
C	8	0.701750	0.943940	-0.494480	2	11	9	7	
C	9	-0.470770	1.875180	-0.339710	1	10	8	22	31
C	10	-1.790500	1.169160	-0.642900	1	9	6	23	32
C	11	1.976450	1.347310	0.209010	1	12	8	24	25
C	12	1.794330	1.197770	1.695270	2	15	13	11	
N	13	2.692970	1.735530	2.564340	9	14	12		
C	14	2.845370	0.914300	3.725000	1	13	16	27	28
N	15	1.358220	-0.054200	2.255420	8	16	12	26	
C	16	1.574470	0.055450	3.659290	1	15	14	29	30
H	17	-3.729890	0.219280	-2.188850	5	1			
H	18	-3.598990	-1.545030	-3.864550	5	2			
H	19	-1.461550	-2.653870	-4.301270	5	3			
H	20	0.529810	-1.984580	-3.095960	5	4			
H	21	1.577030	-0.685140	-1.486070	5	7			
H	22	-0.507160	2.309900	0.686970	5	9			
H	23	-2.127720	0.624470	0.271170	5	10			
H	24	2.212360	2.406930	-0.041890	5	11			
H	25	2.844000	0.722090	-0.104500	5	11			
H	26	0.404460	-0.320420	2.034640	23	15			
H	27	3.767420	0.294220	3.625240	5	14			
H	28	2.902390	1.532480	4.650870	5	14			
H	29	1.693720	-0.949990	4.126110	5	16			
H	30	0.710060	0.586440	4.127380	5	16			
H	31	-0.310280	2.716950	-1.053870	5	9			
H	32	-2.575500	1.924220	-0.886360	5	10			

30napaphen

C	1	-2.766600	-0.372830	-2.124920	2	6	2	17	0	0	0
C	2	-2.725410	-1.371440	-3.021100	2	3	1	18	0	0	0
C	3	-1.547160	-1.909390	-3.371110	2	4	2	19	0	0	0
C	4	-0.410390	-1.448440	-2.825570	2	5	3	20	0	0	0
C	5	-0.445710	-0.446710	-1.926780	2	7	6	4	0	0	0
C	6	-1.629160	0.092060	-1.575220	2	10	5	1	0	0	0
C	7	0.690910	0.019550	-1.376790	2	8	5	21	0	0	0
C	8	0.661980	1.019180	-0.477480	2	11	9	7	0	0	0
C	9	-0.523340	1.549740	-0.130790	2	10	8	22	0	0	0
C	10	-1.661330	1.091410	-0.675010	2	9	6	23	0	0	0
C	11	1.941740	1.537150	0.144840	1	12	8	24	25	0	0
C	12	2.248540	0.841560	1.450370	2	15	13	11	0	0	0
N	13	1.381830	1.037090	2.486900	9	14	12	0	0	0	0
C	14	1.047170	-0.185860	3.146740	1	13	16	27	28	0	0
N	15	2.541790	-0.569770	1.444810	8	16	12	26	0	0	0
C	16	1.449530	-1.219180	2.086250	1	15	14	29	30	0	0
H	17	-3.744990	0.057630	-1.847860	5	1	0	0	0	0	0
H	18	-3.660100	-1.750550	-3.469800	5	2	0	0	0	0	0
H	19	-1.513130	-2.730900	-4.107780	5	3	0	0	0	0	0
H	20	0.549570	-1.903840	-3.126280	5	4	0	0	0	0	0
H	21	1.663520	-0.418660	-1.658590	5	7	0	0	0	0	0
H	22	-0.566180	2.367850	0.608250	5	9	0	0	0	0	0
H	23	-2.620520	1.546380	-0.371230	5	10	0	0	0	0	0
H	24	1.870810	2.634490	0.326930	5	11	0	0	0	0	0
H	25	2.804460	1.394300	-0.545910	5	11	0	0	0	0	0
H	26	2.774270	-0.979630	0.547270	23	15	0	0	0	0	0
H	27	1.655250	-0.288430	4.076310	5	14	0	0	0	0	0
H	28	-0.038800	-0.223170	3.395530	5	14	0	0	0	0	0
H	29	1.761920	-2.198780	2.517060	5	16	0	0	0	0	0
H	30	0.625710	-1.379650	1.349130	5	16	0	0	0	0	0

23norad 1r---noradrenaline 1r--nh2 extended trans configuration

O	1	-2.101786	2.829309	-0.206211	6	7	23	0	0	0	0
O	2	0.284402	3.987758	0.535495	6	8	21	0	0	0	0
O	3	1.206215	-1.841397	-1.382309	6	11	22	0	0	0	0
N	4	-0.186996	-3.674233	0.311043	8	12	19	20	0	0	0
C	5	0.106712	0.033580	-0.340906	2	6	10	11	0	0	0
C	6	-1.009961	0.780989	-0.415123	2	5	7	13	0	0	0
C	7	-0.965802	2.090682	-0.125419	2	1	6	8	0	0	0
C	8	0.188198	2.665727	0.241833	2	2	7	9	0	0	0
C	9	1.306247	1.927664	0.319713	2	8	10	14	0	0	0
C	10	1.261271	0.616537	0.031429	2	5	9	15	0	0	0
C	11	0.057501	-1.446543	-0.664620	1	3	5	12	16	0	0
C	12	-0.044620	-2.290181	0.613600	1	4	11	17	18	0	0
H	13	-1.967011	0.320906	-0.713133	5	6	0	0	0	0	0
H	14	2.260151	2.394399	0.620464	5	9	0	0	0	0	0
H	15	2.184354	0.016870	0.102937	5	10	0	0	0	0	0
H	16	-0.804273	-1.674347	-1.336705	5	11	0	0	0	0	0
H	17	-0.940279	-1.974085	1.198386	5	12	0	0	0	0	0
H	18	0.856920	-2.143691	1.254540	5	12	0	0	0	0	0
H	19	-0.259088	-4.220174	1.164420	23	4	0	0	0	0	0
H	20	0.645686	-4.029630	-0.148287	23	4	0	0	0	0	0
H	21	-0.576915	4.403176	0.705453	21	2	0	0	0	0	0
H	22	1.283508	-1.284687	-2.175700	21	3	0	0	0	0	0
H	23	-2.784437	2.511371	0.409100	21	1	0	0	0	0	0

23norad1s-noradrenaline 1s configuration non nh2 extended configuration

O	1	-2.175561	2.362165	-0.626468	6	7	23	0	0	0	0
O	2	-0.064869	3.812963	0.383406	6	8	21	0	0	0	0
H	3	1.615533	-1.875018	-0.809874	5	11	0	0	0	0	0
N	4	0.537179	-2.306012	1.644630	8	12	19	20	0	0	0
C	5	0.356418	-0.139723	-0.412729	2	6	10	11	0	0	0
C	6	-0.824785	0.461706	-0.644551	2	5	7	13	0	0	0
C	7	-0.978814	1.769216	-0.383883	2	1	6	8	0	0	0
C	8	0.039552	2.486964	0.111173	2	2	7	9	0	0	0
C	9	1.220943	1.895319	0.345532	2	8	10	14	0	0	0
C	10	1.374673	0.586908	0.084282	2	5	9	15	0	0	0
C	11	0.534853	-1.616975	-0.701305	1	3	5	12	16	0	0
C	12	-0.096910	-2.499535	0.384558	1	4	11	17	18	0	0
H	13	-1.672144	-0.116994	-1.048574	5	6	0	0	0	0	0
H	14	2.064427	2.480149	0.751403	5	9	0	0	0	0	0
H	15	2.348571	0.108372	0.283279	5	10	0	0	0	0	0
O	16	-0.051823	-1.951118	-1.940444	6	11	22	0	0	0	0
H	17	0.016678	-3.573569	0.105594	5	12	0	0	0	0	0
H	18	-1.187570	-2.285962	0.482944	5	12	0	0	0	0	0
H	19	0.125445	-2.912763	2.347359	23	4	0	0	0	0	0
H	20	0.369167	-1.367084	1.992218	23	4	0	0	0	0	0
H	21	-0.984479	4.124051	0.411941	21	2	0	0	0	0	0
H	22	0.330544	-1.380187	-2.628431	21	16	0	0	0	0	0
H	23	-2.897032	1.937125	-0.132060	21	1	0	0	0	0	0

31rx821002s active form (rx 58)

C	1	2.720660	-0.348550	2.962740	2	6	2	18	0	0	0
C	2	2.049340	-0.824490	1.902200	2	19	3	1	0	0	0
C	3	1.317860	0.001440	1.136140	2	7	4	2	0	0	0
C	4	1.260000	1.312550	1.431370	2	10	5	3	0	0	0
C	5	1.931610	1.786490	2.493860	2	20	6	4	0	0	0
C	6	2.661350	0.959330	3.259250	2	21	5	1	0	0	0
O	7	0.585030	-0.583170	-0.040760	1	8	3	0	0	0	0
C	8	-0.531390	0.310350	-0.576480	1	13	11	9	7	0	0
C	9	0.034380	1.722270	-0.751270	1	23	22	10	8	0	0
O	10	0.450470	2.277420	0.607040	1	9	4	0	0	0	0
O	11	-1.696610	0.251990	0.414360	1	12	8	0	0	0	0
C	12	-2.869140	1.185560	0.132480	1	26	25	24	11	0	0
C	13	-0.968930	-0.292510	-1.891830	3	17	14	8	0	0	0
N	14	-0.397810	0.123530	-3.228700	1	15	13	0	0	0	0
C	15	-1.355950	-0.548010	-4.213990	1	28	27	16	14	0	0
C	16	-1.877300	-1.797300	-3.492640	1	30	29	17	15	0	0
N	17	-1.993990	-1.397310	-2.018990	1	31	16	13	0	0	0
H	18	3.319880	-1.031200	3.590030	5	1	0	0	0	0	0
H	19	2.097750	-1.899630	1.658930	5	2	0	0	0	0	0
H	20	1.882580	2.861180	2.738910	5	5	0	0	0	0	0
H	21	3.211530	1.353940	4.131110	5	6	0	0	0	0	0
H	22	-0.712200	2.410790	-1.208120	5	9	0	0	0	0	0
H	23	0.931080	1.708550	-1.413670	5	9	0	0	0	0	0
H	24	-3.206000	1.113110	-0.926050	5	12	0	0	0	0	0
H	25	-2.599970	2.241010	0.360680	5	12	0	0	0	0	0
H	26	-3.722380	0.901610	0.787760	5	12	0	0	0	0	0
H	27	-0.836370	-0.794840	-5.168790	5	15	0	0	0	0	0
H	28	-2.189350	0.161520	-4.428910	5	15	0	0	0	0	0
H	29	-2.860360	-2.138430	-3.892650	5	16	0	0	0	0	0
H	30	-1.138470	-2.626510	-3.603450	5	16	0	0	0	0	0
H	31	-1.660120	-2.562320	-1.094970	1	17	0	0	0	0	0

28rx781094--s form (rx59)

C	1	-3.380390	-0.829300	1.543630	2	17	6	2	0	0	0
C	2	-3.891970	0.369020	1.872350	2	18	3	1	0	0	0
C	3	-3.108960	1.462090	1.882330	2	19	4	2	0	0	0
C	4	-1.806950	1.367340	1.563490	2	20	5	3	0	0	0
C	5	-1.300940	0.170350	1.235580	2	7	6	4	0	0	0
C	6	-2.081760	-0.919240	1.224560	2	10	5	1	0	0	0
O	7	0.001870	-0.018060	0.896030	6	8	5	0	0	0	0
C	8	0.032080	-0.646150	-0.373640	1	12	11	9	7	0	0
C	9	-0.814610	-1.935500	-0.348550	1	22	21	10	8	0	0
O	10	-1.481460	-2.090790	0.889770	6	9	6	0	0	0	0
H	11	-0.381900	0.083530	-1.112660	5	8	0	0	0	0	0
C	12	1.465850	-0.908140	-0.766280	2	16	13	8	0	0	0
N	13	1.753450	-1.601270	-1.902350	9	14	12	0	0	0	0
C	14	2.971020	-1.151160	-2.500450	1	26	25	15	13	0	0
C	15	3.675260	-0.430720	-1.338480	1	28	27	16	14	0	0
C	16	2.491150	0.182560	-0.577620	1	12	15	23	24	0	0
H	17	-4.018530	-1.729200	1.536500	5	1	0	0	0	0	0
H	18	-4.960220	0.455800	2.136530	5	2	0	0	0	0	0
H	19	-3.537380	2.442520	2.153760	5	3	0	0	0	0	0
H	20	-1.160700	2.261440	1.569230	5	4	0	0	0	0	0
H	21	-1.580230	-1.951370	-1.160930	5	9	0	0	0	0	0
H	22	-0.184660	-2.848830	-0.449710	5	9	0	0	0	0	0
H	23	2.146360	1.118400	-1.077800	5	16	0	0	0	0	0
H	24	2.711510	0.382240	0.496750	5	16	0	0	0	0	0
H	25	2.735780	-0.443620	-3.330030	5	14	0	0	0	0	0
H	26	3.563860	-2.007230	-2.898230	5	14	0	0	0	0	0
H	27	4.193780	-1.177740	-0.689200	5	15	0	0	0	0	0
H	28	4.423560	0.325120	-1.676140	5	15	0	0	0	0	0

```
27rx781094 —  r form   (rx59r)
 C    1   -7.721670   -5.784710    8.945150    2   17    6    2    0    0    0
 C    2   -8.203560   -4.829430    9.756950    2   18    3    1    0    0    0
 C    3   -7.700750   -3.584900    9.705610    2   19    4    2    0    0    0
 C    4   -6.715370   -3.291250    8.841450    2   20    5    3    0    0    0
 C    5   -6.236310   -4.246110    8.027570    2    7    6    4    0    0    0
 C    6   -6.733180   -5.491360    8.084740    2   10    5    1    0    0    0
 O    7   -5.224730   -3.877310    7.195130    6    8    5    0    0    0    0
 C    8   -5.093120   -4.786290    6.118780    1   12   11    9    7    0    0
 C    9   -5.046310   -6.197790    6.725150    1   22   21   10    8    0    0
 O   10   -6.307130   -6.504100    7.280990    6    9    6    0    0    0    0
 H   11   -3.830960   -4.587690    5.500920    5    8    0    0    0    0    0
 C   12   -6.241580   -4.655440    5.141430    2   16   13    8    0    0    0
 N   13   -6.366440   -5.492150    4.074960    9   14   12    0    0    0    0
 C   14   -7.000360   -4.832640    2.976700    1   24   23   15   13    0    0
 C   15   -7.685040   -3.655020    3.635260    1   26   25   16   14    0    0
 N   16   -6.789550   -3.381700    4.759780    8   27   15   12    0    0    0
 H   17   -8.138710   -6.805750    8.986720    5    1    0    0    0    0    0
 H   18   -9.014690   -5.067230   10.466920    5    2    0    0    0    0    0
 H   19   -8.097730   -2.802150   10.375100    5    3    0    0    0    0    0
 H   20   -6.301730   -2.268680    8.803270    5    4    0    0    0    0    0
 H   21   -4.851470   -6.972030    5.947400    5    9    0    0    0    0    0
 H   22   -4.270910   -6.297690    7.522390    5    9    0    0    0    0    0
 H   23   -7.722780   -5.508920    2.463580    5   14    0    0    0    0    0
 H   24   -6.225980   -4.484170    2.253130    5   14    0    0    0    0    0
 H   25   -7.812950   -2.759380    3.033790    5   15    0    0    0    0    0
 H   26   -8.676290   -3.962620    4.098820    5   15    0    0    0    0    0
 H   27   -7.235940   -2.859770    5.506310   23   16    0    0    0    0    0
```

27SKF86466

C	1	-0.734620	1.924140	-1.174100	2	12	6	2	0	0	0
C	2	-1.404440	1.801620	-2.333210	2	14	3	1	0	0	0
C	3	-1.745880	0.592570	-2.793580	2	15	4	2	0	0	0
C	4	-1.402910	-0.493750	-2.090400	2	16	5	3	0	0	0
C	5	-0.728070	-0.394660	-0.927870	2	7	6	4	0	0	0
C	6	-0.394760	0.829230	-0.453440	2	11	5	1	0	0	0
C	7	-0.366680	-1.707430	-0.248870	1	18	17	8	5	0	0
C	8	1.010980	-1.716460	0.425860	1	20	19	9	7	0	0
N	9	0.996720	-1.212650	1.757880	8	13	10	8	0	0	0
C	10	0.172290	-0.053170	1.938270	1	22	21	11	9	0	0
C	11	0.345150	1.029210	0.864480	1	24	23	10	6	0	0
CL	12	-0.327280	3.592500	-0.676140	12	1	0	0	0	0	0
C	13	2.325640	-1.065540	2.301180	1	27	26	25	9	0	0
H	14	-1.680870	2.695540	-2.919240	5	2	0	0	0	0	0
H	15	-2.296680	0.492320	-3.745180	5	3	0	0	0	0	0
H	16	-1.684390	-1.483510	-2.488720	5	4	0	0	0	0	0
H	17	-1.176400	-2.012650	0.454050	5	7	0	0	0	0	0
H	18	-0.334960	-2.513880	-1.019990	5	7	0	0	0	0	0
H	19	1.372270	-2.770970	0.487270	5	8	0	0	0	0	0
H	20	1.740340	-1.162630	-0.212420	5	8	0	0	0	0	0
H	21	0.372700	0.375010	2.949470	5	10	0	0	0	0	0
H	22	-0.897330	-0.361100	1.991220	5	10	0	0	0	0	0
H	23	1.423310	1.212990	0.649630	5	11	0	0	0	0	0
H	24	-0.040930	1.953910	1.351830	5	11	0	0	0	0	0
H	25	2.894540	-0.262820	1.778230	5	13	0	0	0	0	0
H	26	2.887330	-2.023150	2.209060	5	13	0	0	0	0	0
H	27	2.282220	-0.828090	3.388510	5	13	0	0	0	0	0

23tiamenidine

N	1	-2.262950	-1.838620	0.213550	8	5	2	19	
C	2	-3.507810	-2.447860	0.564750	1	3	1	15	20
C	3	-3.119090	-3.356610	1.737750	1	4	2	14	16
N	4	-2.130300	-2.589410	2.435000	8	17	5	3	
C	5	-1.491780	-1.791610	1.424930	2	11	4	1	
C	6	0.513810	-0.906070	2.530450	2	11	10	7	
C	7	0.433370	-1.455810	3.753760	2	18	6	8	
S	8	1.797050	-0.949710	4.759810	15	7	9		
C	9	2.396890	0.003460	3.397390	2	10	12	8	
C	10	1.583290	-0.111120	2.332820	2	9	6	13	
N	11	-0.358860	-1.081420	1.517480	9	6	5		
H	12	3.313940	0.613880	3.406570	5	9			
C	13	1.846790	0.594930	1.028140	1	10	21	22	23
H	14	-3.976700	-3.617500	2.401960	5	3			
H	15	-4.231750	-1.664920	0.897410	5	2			
H	16	-2.643600	-4.297320	1.370400	5	3			
H	17	-2.580370	-2.023550	3.149660	23	4			
H	18	-0.364450	-2.132100	4.093620	5	7			
H	19	-2.410160	-0.941810	-0.238550	23	1			
H	20	-3.929220	-3.004630	-0.304430	5	2			
H	21	2.025460	-0.146000	0.215820	5	13			
H	22	0.979550	1.234070	0.744830	5	13			
H	23	2.742230	1.254820	1.084200	5	13			

48wy26392 (wy26392a)

C	1	-2.205210	0.825480	-5.796270	2	23	6	2	0	0	0
C	2	-3.203560	1.107780	-6.647630	2	24	3	1	0	0	0
C	3	-4.403680	0.533370	-6.483780	2	25	4	2	0	0	0
C	4	-4.590530	-0.324230	-5.469950	2	26	5	3	0	0	0
C	5	-3.588720	-0.607140	-4.617820	2	14	6	4	0	0	0
C	6	-2.380400	-0.027430	-4.767980	2	7	5	1	0	0	0
C	7	-1.217550	-0.323160	-3.821820	1	27	12	8	6	0	0
C	8	-0.470960	0.954980	-3.369760	1	29	28	9	7	0	0
C	9	0.360760	0.710470	-2.093530	1	30	15	10	8	0	0
C	10	-0.638620	0.291500	-0.990190	1	32	31	11	9	0	0
C	11	-1.910870	-0.376420	-1.537550	1	34	33	12	10	0	0
N	12	-1.572170	-1.149140	-2.691920	8	13	11	7	0	0	0
C	13	-2.505300	-2.177560	-3.027030	1	36	35	14	12	0	0
C	14	-3.835550	-1.595880	-3.505680	1	38	37	13	5	0	0
N	15	1.172260	1.842530	-1.631660	8	21	16	9	0	0	0
S	16	2.342200	1.410320	-0.469050	18	15	17	22	18	0	0
O	17	3.430600	0.768970	-1.015650	7	16	0	0	0	0	0
C	18	2.879310	2.959980	0.330550	1	16	19	39	40	0	0
C	19	3.880670	2.721000	1.472530	1	42	41	20	18	0	0
C	20	4.313500	4.040310	2.126840	1	45	44	43	19	0	0
C	21	1.742260	2.618560	-2.703840	1	48	47	46	15	0	0
O	22	1.854230	0.612550	0.542760	7	16	0	0	0	0	0
H	23	-1.227000	1.305720	-5.958810	5	1	0	0	0	0	0
H	24	-3.037390	1.810340	-7.482840	5	2	0	0	0	0	0
H	25	-5.229060	0.760460	-7.180730	5	3	0	0	0	0	0
H	26	-5.576970	-0.801330	-5.340480	5	4	0	0	0	0	0
H	27	-0.500700	-0.941400	-4.414690	5	7	0	0	0	0	0
H	28	0.183440	1.272570	-4.213630	5	8	0	0	0	0	0
H	29	-1.195710	1.779950	-3.171360	5	8	0	0	0	0	0
H	30	1.033780	-0.146820	-2.345910	5	9	0	0	0	0	0
H	31	-0.146600	-0.437210	-0.304060	5	10	0	0	0	0	0
H	32	-0.938640	1.175910	-0.378510	5	10	0	0	0	0	0
H	33	-2.345000	-1.024260	-0.739230	5	11	0	0	0	0	0
H	34	-2.684900	0.385120	-1.795450	5	11	0	0	0	0	0
H	35	-2.057490	-2.815030	-3.826320	5	13	0	0	0	0	0
H	36	-2.659000	-2.852550	-2.152150	5	13	0	0	0	0	0
H	37	-4.376910	-1.084410	-2.675840	5	14	0	0	0	0	0
H	38	-4.486290	-2.430150	-3.860810	5	14	0	0	0	0	0
H	39	3.355050	3.624040	-0.425440	5	18	0	0	0	0	0
H	40	1.971640	3.474110	0.723650	5	18	0	0	0	0	0
H	41	4.786170	2.196650	1.082570	5	19	0	0	0	0	0
H	42	3.424700	2.066500	2.253770	5	19	0	0	0	0	0
H	43	5.040180	3.858540	2.952480	5	20	0	0	0	0	0
H	44	3.439250	4.580690	2.557670	5	20	0	0	0	0	0
H	45	4.804010	4.714520	1.387410	5	20	0	0	0	0	0
H	46	2.370480	3.457720	-2.333500	5	21	0	0	0	0	0
H	47	0.938140	3.133570	-3.274780	5	21	0	0	0	0	0
H	48	2.357830	1.988920	-3.388520	5	21	0	0	0	0	0

53wy27127 (wy27127a)

C	1	-1.571360	-3.880540	0.354100	2	23	6	2	
C	2	-2.206750	-5.055620	0.224490	2	24	3	1	
C	3	-3.248470	-5.343010	1.017890	2	25	4	2	
C	4	-3.641020	-4.450760	1.938900	2	26	5	3	
C	5	-3.003000	-3.273310	2.068690	2	14	6	4	
C	6	-1.959730	-2.971170	1.269170	2	7	5	1	
C	7	-1.210810	-1.643810	1.381860	1	27	12	8	6
C	8	-0.920780	-0.995990	0.005950	1	29	28	9	7
C	9	-0.697950	0.517640	0.154480	1	30	15	10	8
C	10	-1.978290	1.171850	0.702820	1	32	31	11	9
C	11	-2.744700	0.200000	1.620970	1	34	33	12	10
N	12	-1.833580	-0.692440	2.281550	8	13	11	7	
C	13	-2.350450	-1.314730	3.460050	1	36	35	14	12
C	14	-3.466050	-2.307260	3.131070	1	38	37	13	5
N	15	-0.067360	1.185430	-0.980750	8	21	16	9	
S	16	-0.958680	1.450590	-2.408310	18	15	17	18	22
O	17	-1.775920	2.559190	-2.335370	7	16			
C	18	-1.988050	0.023760	-2.841730	1	16	39	40	19
H	19	-1.367790	-0.898220	-2.908790	5	18			
C	20	1.575720	3.059500	-1.562730	1	21	41	46	47
C	21	0.631170	2.394630	-0.539510	1	15	20	52	53
O	22	-0.132470	1.629040	-3.503820	7	16			
H	23	-0.714060	-3.670360	-0.305800	5	1			
H	24	-1.872100	-5.785500	-0.533150	5	2			
H	25	-3.775300	-6.307780	0.916830	5	3			
H	26	-4.495010	-4.691090	2.594960	5	4			
H	27	-0.227300	-1.892020	1.848870	5	7			
H	28	-0.035400	-1.464440	-0.486540	5	8			
H	29	-1.805600	-1.192570	-0.632810	5	8			
H	30	0.050220	0.539770	0.983330	5	9			
H	31	-1.705410	2.092760	1.271600	5	10			
H	32	-2.666500	1.492710	-0.111860	5	10			
H	33	-3.317540	0.800720	2.366470	5	11			
H	34	-3.488960	-0.388370	1.033160	5	11			
H	35	-1.513440	-1.840290	3.978600	5	13			
H	36	-2.708770	-0.537760	4.175960	5	13			
H	37	-4.380830	-1.781380	2.770520	5	14			
H	38	-3.745770	-2.856130	4.061710	5	14			
H	39	-2.821350	-0.096770	-2.115270	5	19			
H	40	-2.452800	0.200470	-3.837950	5	18			
H	41	2.394440	4.042240	-0.914160	8	20	42	48	
S	42	3.500740	4.844670	-1.927280	18	41	43	44	45
O	43	2.886560	5.605300	-2.893830	7	42			
O	44	4.391630	3.988510	-2.530100	7	42			
C	45	4.393330	5.929370	-0.778830	1	42	49	50	51
H	46	2.227430	2.274010	-2.014860	5	20			
H	47	0.989980	3.564500	-2.366530	5	20			
H	48	1.807280	4.728850	-0.449690	23	41			
H	49	3.679760	6.630050	-0.289520	5	45			
H	50	4.897090	5.316770	0.002510	5	45			
H	51	5.159860	6.516940	-1.332740	5	45			
H	52	-0.101850	3.149660	-0.166460	5	21			
H	53	1.288220	2.129920	0.322350	5	21			

31xylazine

N	1	-2.296880	-2.986280	1.882470	9	5	2		
C	2	-3.697070	-3.060450	1.661340	1	3	1	16	23
C	3	-4.434840	-1.748180	1.968000	1	4	2	15	17
C	4	-3.957050	-0.616720	1.045580	1	3	18	22	31
C	5	-1.516490	-1.901790	1.697460	2	1	12	31	
C	6	0.560570	-1.428030	3.046830	2	12	11	7	
C	7	0.480890	-1.954440	4.287370	2	19	8	6	
C	8	1.113050	-1.357650	5.313780	2	20	9	7	
C	9	1.823980	-0.238400	5.117110	2	21	10	8	
C	10	1.906760	0.284880	3.886070	2	13	11	9	
C	11	1.280220	-0.302870	2.851680	2	10	6	14	
N	12	-0.111950	-2.049300	1.935520	8	6	5	30	
H	13	2.494560	1.205080	3.727360	5	10			
C	14	1.414910	0.320650	1.478100	1	11	24	25	26
H	15	-5.531660	-1.899920	1.821560	5	3			
H	16	-3.876170	-3.355170	0.601010	5	2			
H	17	-4.288730	-1.468180	3.039220	5	3			
H	18	-4.148440	-0.898070	-0.015800	5	4			
C	19	-0.307620	-3.221540	4.542600	1	7	27	28	29
H	20	1.050350	-1.784140	6.329300	5	8			
H	21	2.339980	0.247980	5.963230	5	9			
H	22	-4.528080	0.319150	1.246890	5	4			
H	23	-4.104520	-3.879190	2.298940	5	2			
H	24	1.262760	-0.410370	0.652410	5	14			
H	25	0.673080	1.142710	1.359510	5	14			
H	26	2.431260	0.750390	1.325220	5	14			
H	27	-0.118770	-3.987750	3.756910	5	19			
H	28	-0.043430	-3.700110	5.512970	5	19			
H	29	-1.397380	-2.993070	4.568160	5	19			
H	30	0.299170	-2.917870	1.610790	23	12			
S	31	-2.175450	-0.330580	1.297610	15	4	5		

31xylazinea

N	1	-2.101560	-3.024250	1.714320	9	5	2	0	0	0	0
C	2	-3.479550	-3.288920	1.503610	1	3	1	16	23	0	0
C	3	-4.362970	-2.035670	1.598960	1	4	2	15	17	0	0
C	4	-3.989190	-1.012460	0.515820	1	3	18	22	31	0	0
C	5	-1.440860	-1.898540	1.374420	2	1	12	31	0	0	0
C	6	0.528450	-1.014360	2.679970	2	12	11	7	0	0	0
C	7	1.223200	0.088900	2.331020	2	19	8	6	0	0	0
C	8	1.758230	0.877830	3.279470	2	20	9	7	0	0	0
C	9	1.607290	0.576640	4.576810	2	21	10	8	0	0	0
C	10	0.920800	-0.520230	4.926620	2	13	11	9	0	0	0
C	11	0.380690	-1.317010	3.987250	2	10	6	14	0	0	0
N	12	-0.035910	-1.851250	1.653320	8	6	5	30	0	0	0
H	13	0.802870	-0.762730	5.996400	5	10	0	0	0	0	0
C	14	-0.378190	-2.553360	4.420330	1	11	24	25	26	0	0
H	15	-5.432880	-2.329360	1.470490	5	3	0	0	0	0	0
H	16	-3.603210	-3.762710	0.501890	5	2	0	0	0	0	0
H	17	-4.273730	-1.580600	2.614950	5	3	0	0	0	0	0
H	18	-4.118970	-1.473580	-0.490570	5	4	0	0	0	0	0
C	19	1.421970	0.448030	0.873410	1	7	27	28	29	0	0
H	20	2.326330	1.780410	2.997010	5	8	0	0	0	0	0
H	21	2.047950	1.226860	5.352570	5	9	0	0	0	0	0
H	22	-4.666310	-0.128320	0.563450	5	4	0	0	0	0	0
H	23	-3.807140	-4.039190	2.260360	5	2	0	0	0	0	0
H	24	-1.474830	-2.369450	4.357300	5	14	0	0	0	0	0
H	25	-0.120490	-3.434610	3.790260	5	14	0	0	0	0	0
H	26	-0.149480	-2.847310	5.469950	5	14	0	0	0	0	0
H	27	0.521620	0.974160	0.483250	5	19	0	0	0	0	0
H	28	2.298080	1.118350	0.719360	5	19	0	0	0	0	0
H	29	1.606700	-0.453560	0.246240	5	19	0	0	0	0	0
H	30	0.469420	-2.712860	1.478110	23	12	0	0	0	0	0
S	31	-2.257850	-0.487790	0.738500	15	4	5	0	0	0	0

52yohimbine

C	1	-2.958449	0.401570	-5.905529	2	27	6	2	0	0	0
C	2	-4.262139	0.333100	-6.227240	2	28	3	1	0	0	0
C	3	-5.167399	-0.113120	-5.336990	2	4	2	51	0	0	0
C	4	-4.786520	-0.499580	-4.106781	2	5	3	52	0	0	0
C	5	-3.485569	-0.426150	-3.797210	2	7	6	4	0	0	0
C	6	-2.574810	0.018080	-4.679960	2	9	5	1	0	0	0
C	7	-2.853820	-0.743600	-2.654300	2	10	8	5	0	0	0
C	8	-1.543990	-0.495570	-2.804671	2	13	9	7	0	0	0
N	9	-1.246879	0.002800	-4.122480	8	29	8	6	0	0	0
C	10	-3.419250	-1.291441	-1.382350	1	31	30	11	7	0	0
C	11	-2.289299	-1.976870	-0.597600	1	33	32	12	10	0	0
N	12	-1.144290	-1.110530	-0.467660	8	14	13	11	0	0	0
C	13	-0.536070	-0.740070	-1.715000	1	34	17	12	8	0	0
C	14	-0.175670	-1.611610	0.475590	1	36	35	15	12	0	0
C	15	1.179970	-0.869850	0.431200	1	37	18	16	14	0	0
C	16	1.008010	0.558620	-0.105910	1	38	21	17	15	0	0
C	17	0.312921	0.522880	-1.484730	1	40	39	16	13	0	0
C	18	1.879810	-0.922080	1.807450	1	42	41	19	15	0	0
C	19	2.902470	0.205020	2.024660	1	44	43	20	18	0	0
C	20	3.434330	0.699110	0.680070	1	45	22	21	19	0	0
C	21	2.327240	1.371310	-0.151910	1	46	23	20	16	0	0
O	22	4.533090	1.566180	0.849990	6	47	20	0	0	0	0
C	23	2.029120	2.829350	0.196530	3	26	24	21	0	0	0
O	24	1.181250	3.499200	-0.604000	6	25	23	0	0	0	0
C	25	1.796330	4.310440	-1.580040	1	50	49	48	24	0	0
O	26	2.516420	3.389930	1.151140	7	23	0	0	0	0	0
H	27	-2.214089	0.765960	-6.633320	5	1	0	0	0	0	0
H	28	-4.592730	0.646050	-7.232841	5	2	0	0	0	0	0
H	29	-0.794050	0.911560	-4.125530	23	9	0	0	0	0	0
H	30	-4.236060	-2.020810	-1.593710	5	10	0	0	0	0	0
H	31	-3.843620	-0.444730	-0.793160	5	10	0	0	0	0	0
H	32	-1.988400	-2.923960	-1.107520	5	11	0	0	0	0	0
H	33	-2.680099	-2.244560	0.412920	5	11	0	0	0	0	0
H	34	0.102480	-1.583520	-2.073790	5	13	0	0	0	0	0
H	35	-0.641630	-1.500930	1.481430	5	14	0	0	0	0	0
H	36	0.009211	-2.700900	0.314340	5	14	0	0	0	0	0
H	37	1.837710	-1.387810	-0.309630	5	15	0	0	0	0	0
H	38	0.319970	1.041690	0.630390	5	16	0	0	0	0	0
H	39	-0.326509	1.433360	-1.573020	5	17	0	0	0	0	0
H	40	1.054740	0.575360	-2.315480	5	17	0	0	0	0	0
H	41	2.377290	-1.916360	1.909220	5	18	0	0	0	0	0
H	42	1.139010	-0.861600	2.638910	5	18	0	0	0	0	0
H	43	3.736380	-0.149730	2.676510	5	19	0	0	0	0	0
H	44	2.420680	1.061110	2.553510	5	19	0	0	0	0	0
H	45	3.858660	-0.171020	0.124090	5	20	0	0	0	0	0
H	46	2.731880	1.409490	-1.190330	5	21	0	0	0	0	0
H	47	4.354240	2.176760	1.582600	21	22	0	0	0	0	0
H	48	2.427850	3.678570	-2.246240	5	25	0	0	0	0	0
H	49	2.398850	5.103110	-1.079360	5	25	0	0	0	0	0
H	50	0.980310	4.779280	-2.174230	5	25	0	0	0	0	0
H	51	-6.233540	-0.162260	-5.618780	5	3	0	0	0	0	0
H	52	-5.528230	-0.863650	-3.376040	5	4	0	0	0	0	0